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13. ABSTRACT (Maximum 200 words)

The research supported by this grant included two projects: *I. Temperature Control In Polymer Extrusion Processes*, here an optimization problem was formulated. This problem was motivated by the desire to obtain uniform extrudate temperature at the die exit in a polymer extrusion process. Control was effected by adjustments to the heat flux along the surface of the pipe. An optimality system of partial differential equations was derived from which optimal controls and states may be determined. Then, finite element discretizations of the optimality system were defined and error estimates were provided along with an efficient solution algorithm for the discreet. Finally, computational results were given for a model example with Oldroyd type fluid, demonstrating the effectiveness of our theory and

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Final Report

To

Army Research Office

for the Proposal

COMPUTATIONAL METHODS FOR THE SIMULATION OF NON-NEWTONIAN FLOWS

ABSTRACT

The research supported by this grant included two projects: *I. Temperature Control In Polymer Extrusion Processes*, here an optimization problem was formulated. This problem was motivated by the desire to obtain uniform extrudate temperature at the die exit in a polymer extrusion process. Control was effected by adjustments to the heat flux along the surface of the pipe. An optimality system of partial differential equations was derived from which optimal controls and states may be determined. Then, finite element discretizations of the optimality system were defined and error estimates were provided along with an efficient solution algorithm for the discreet. Finally, computational results were given for a model example with Oldroyd type fluid, demonstrating the effectiveness of our theory and methods, as well as their potential applicability to industrial problems. *II. Analysis and Finite Element Approximation of An Optimal Control Problem in Electrochemistry with Current Density Controls*, here an optimal control problem for impressed cathodic systems in electrochemistry was studied. The control in this problem was the current density on the anode. A matching objective functional was considered. The existence of an optimal solution was proved. The use of Lagrange multiplier rules was justified and an optimality system of equations established. Finally, a finite element algorithm was defined and optimal error estimates were derived.

Temperature Control In Polymer Extrusion Processes

In polymer extrusion processes, one is often interested in maintaining a quasi-uniform temperature, to reduce material (extrusion product) inhomogeneity, throughout the extrudate cooling process. In this project, we studied the somewhat simplified case: one tries to obtain a uniform temperature distribution at the exit under a steady state situation. The means by which we achieved such a uniform temperature distribution at the exit were to adjust the heat flux on the surface of the pipe near the exit.

The extrudate in equation was assumed to be a viscoelastic fluid of the Oldroyd type such as polymer melts with a fast relaxation mode. We took as the governing equations for the Oldroyd type the Navier-Stokes equations, the incompressibility constraint, the appropriate constitutive equation for an Oldroyd model, the energy equation, and simplified boundary conditions. The control function was determined in a manner that would allow hot spots to be avoided.

We investigated two means of obtaining a uniform temperature distribution. The first is to make the gradient of the temperature along a portion of the boundary small. Another means of achieving the desired result is to try to force the temperature field itself to be quasi-uniform. Numerical experiments revealed that both techniques work effectively for the desired objective. However, we focus our research on the latter.

We proved the existence and uniqueness of optimal solutions and derived an optimality system, that is, a set of equations from which the optimal control and state may be determined. Also, finite element methods and numerical examples were presented. We also developed an iterative algorithm to compute the approximate solution. The convergence of our algorithm was proved and a comparison with a direct method made.

Analysis and Finite Element Approximation of an Optimal Control Problem in Electrochemistry with Current Density Controls

We investigated an optimal control problem for impressed cathodic systems. A typical example of an impressed cathodic system is a metal container filled with an electrolyte. The painted portion of the container surface is usually treated as insulated. The unpainted apart is divided into cathode and anode that are connected to the negative and positive poles of an electrical source, respectively. By adjusting the current density on the anode we could effectively alter the potential distribution on the entire bounding surface or in the entire flow domain. The potential distribution, of course, affects on the chemical reaction process occurring inside the flow domain, which in turn affect the rate of corrosion of the metal container. Thus, the current density on the anode can be used as a practical control variable for generation a desired potential field. This idea can be conveniently formulated as optimal control problems for the potential equation with appropriate boundary conditions. Optimal control problems of this sort have been studied. Here existence of an optimal solution is proved. The use of Lagrange multiplier rules is justified and an optimality system of equations is established. Finally, a finite element algorithm is defined and optimal error estimates are derived.

COMPUTATIONAL ONR-NON NEWTONIA FLOW
ARMY RESEARCH (5-24694)

	BALANCES
SALARIES & WAGES	$12,498
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BRIEF OUTLINE OF RESEARCH FINDINGS

Abstract. An optimization problem is formulated motivated by the desire to obtain uniform extrudate temperature at the die exit in a polymer extrusion process. Control is effected by adjustments to the heat flux along the surface of the pipe. An optimality system of partial differential equations is derived from which optimal controls and states may be determined. Then, finite element discretizations of the optimality system are defined and error estimates are provided along with an efficient solution algorithm for the discrete equations. Finally, computational results are given for a model example with Oldroyd type fluid, demonstrating the effectiveness of our theory and method as well as their potential applicability to industrial problems.

BRIEF OUTLINE OF RESEARCH FINDINGS

In polymer extrusion processes, one is often interested in maintaining a quasi-uniform temperature, so as to reduce material (extrusion product) inhomegeneity, throughout the extrudate cooling process. In this research, we study how one obtains a uniform temperature distribution at the exit under a steady state situation. The means we use to achieve such a uniform temperature distribution at the exit, is to adjust the heat flux on the surface of the pipe near the exit.

The extrude in question is assumed to be a viscoelastic fluid of the Oldroyd type, such as polymer melts with a fast relaxation mode. Two means of obtaining a uniform temperature distribution, resulting in two different functionals, have been investigated. The first involves making the gradient of the temperature along the boundary small. Thus, for example, given a velocity field , we seek a temperature field and a control field such that the functional

$$M(T,g) = \frac{\alpha}{2}\int_{\Gamma_0} |\mathrm{grad}_s T|^2 d\Gamma + \frac{\kappa\delta}{2}\int_{\Gamma_c} |g|^2 d\Gamma$$

is minimized subject, of course, to the constraints imposed by the flow equations. Here the minimization results in a quasi-uniform temperature distribution along the boundary segment, since the surface derivatives of the temperature are forced to be small. Another means of achieving the desired result is to try to directly force the temperature field itself to be quasi-uniform. Thus, now, given a velocity field, we would seek a temperature field and a control field such that the second functional

$$N(T,g) = \frac{1}{2\gamma}\int_{\Gamma_0} |T - T_d|^2 d\Gamma + \frac{\kappa\delta}{2}\int_{\Gamma_c} |g|^2 d\Gamma$$

is minimized subject to the constraints imposed by the flow equations. The non-negative parameters γ and δ can be used to change the relative importance of the two terms appearing in the definition of N as well as to act as penalty parameters. Our numerical experiments demonstrated that a small γ is more useful in achieving quasi-uniform boundary temperature distributions, although it also reduces the accuracy of the approximate solution. Numerical experiments also show that both M and N work effectively for the desired objective. However, our work has focused on N. Under the realistic assumption that $u \cdot n = o$ on the boundary, we have proved the existence and uniqueness of optimal solutions and derived an optimality system, i.e., a set of equations from which the optimal control and state may be determined. In addition, finite element methods have been used to compute an approximate solution of the optimality system. Optimal error estimates have been derived and numerical experiments have been performed. Finally, we have developed an iterating algorithm to compute the approximate solution. The convergence of our algorithm has been proved and a comparison with the direct method made.

Control problems for the fully coupled problem as well as temperature matching for the entire extrudate will be addressed next.

Temperature Control In Polymer Extrusion Processes†

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Abstract. An optimization problem is formulated motivated by the desire to obtain uniform extrudate temperature at the die exit in a polymer extrusion process. Control is effected by adjustments to the heat flux along the surface of the pipe. An optimality system of partial differential equations is derived from which optimal controls and states may be determined. Then, finite element discretizations of the optimality system are defined and error estimates are provided along with an efficient solution algorithm for the discrete equations. Finally, computational results are given for a model example with Oldroyd type fluid, demonstrating the effectiveness of our theory and method as well as their potential applicability to industrial problems.

1. Introduction

In polymer extrusion processes, one is often interested in maintaining a quasi-uniform temperature, so as to reduce material (extrusion product) inhomogeneity, throughout the extrudate cooling process. In this paper, we will study the somewhat simplified case: one tries to obtain a uniform temperature distribution at the exit under steady state situation. The means we use to achieve such a uniform temperature distribution at the exit is to adjust the heat flux on the surface of the pipe near the exit.

The extrudate in question will be assumed to be viscoelastic fluid of Oldroyd type such as polymer melts with a fast relaxation mode [10]. Let $\mathbf{u}$ denote the velocity field, p the pressure field, T the temperature field and $\boldsymbol{\tau}$ the purely elastic part of the extra stress. Let $\mathbf{D} = \frac{1}{2}(\operatorname{grad}\mathbf{u} + \operatorname{grad}\mathbf{u}^T)$, $\mathbf{W} = \frac{1}{2}(\operatorname{grad}\mathbf{u} - \operatorname{grad}\mathbf{u}^T)$ and $D_a\boldsymbol{\tau} = (\mathbf{u}\cdot\operatorname{grad})\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{W} - \mathbf{W}\boldsymbol{\tau} - a(\mathbf{D}\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{D})$ where $-1 \le a \le 1$. The parameters Re, We and ω are the Reynolds number, Weissenberg number and retardation parameter, respectively. The governing equations for the Oldroyd type fluid, in dimensionless form, is given by the Navier-Stokes equations

$$Re(\mathbf{u}\cdot\operatorname{grad})\mathbf{u} + \operatorname{grad} p = (1-\omega)\Delta\mathbf{u} + \operatorname{div}\boldsymbol{\tau} + \mathbf{f}\,, \quad \text{in } \Omega\,, \tag{1.1}$$

the incompressiblity constraint

$$\operatorname{div}\mathbf{u} = 0 \quad \text{in } \Omega\,, \tag{1.2}$$

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the constitutive equation (Oldroyd model)

$$\boldsymbol{\tau} + We D_a \boldsymbol{\tau} = 2\omega \mathbf{D} \quad \text{in } \Omega\,, \tag{1.3}$$

and, for simplicity, the boundary condition

$$\mathbf{u} = \mathbf{h} \quad \text{on } \Gamma\,, \tag{1.4}$$

and also the energy equation

$$\begin{aligned} -\kappa\,\Delta T + (\mathbf{u}\cdot\mathbf{grad}\,)T \\ = \bar{Q} + 2\mu(\mathbf{grad}\,\mathbf{u} + \mathbf{grad}\,\mathbf{u}^T) : (\mathbf{grad}\,\mathbf{u} + \mathbf{grad}\,\mathbf{u}^T) \quad \text{in } \Omega\,, \end{aligned} \tag{1.5}$$

with boundary conditions

$$T = 0 \quad \text{on } \Gamma_D\,, \tag{1.6}$$

$$\frac{\partial T}{\partial n} = H_N \quad \text{on } \Gamma_N \cup \Gamma_O\,, \tag{1.7}$$

$$\frac{\partial T}{\partial n} = g \quad \text{on } \Gamma_C\,. \tag{1.8}$$

The data functions $\mathbf{f}$, $\bar{Q}$, H_N, and $\mathbf{h}$ are assumed known; the control g is to be determined so that hot spots are avoided. The constants κ and μ depend on the thermal conductivity coefficient, density, specific heat at constant volume, and viscosity coefficient of the fluid. See [11] for details. We assumed that buoyancy effects can be negelected, and thus the temperature variable does not appear in (1.1).

Two means of obtaining a uniform temperature distribution come to mind. The first is to make the gradient of the temperature along the boundary Γ_o small. Thus, for example, given a velocity field $\mathbf{u}$, we would seek a temperature field T and a control field g such that the functional

$$\mathcal{M}(T,g) = \frac{\alpha}{2}\int_{\Gamma_O} |\mathbf{grad}_s\, T|^2\, d\Gamma + \frac{\kappa\delta}{2}\int_{\Gamma_C} |g|^2\, d\Gamma \tag{1.9}$$

is minimized subject, of course, to the constraints imposed by the flow equations (1.5)-(1.8). Here, $\mathbf{grad}_s$ denotes the surface gradient operator, *e.g.*, in $\mathbf{R}^2$, the tangential derivative operator $\partial/\partial\tau$. The non-negative parameters α and δ can be used to change the relative importance of the the two terms appearing in the definition of $\mathcal{M}$ as well as to act as penalty parameters. The appearance of the control g in the definition of $\mathcal{J}$ is necessary because we are not imposing any *a priori* limits on the size of this control. The minimization of (1.9) results in a quasi-uniform temperature distribution along the boundary segment Γ_o because the surface derivatives of the temperature are forced to be small. Another means of achieving the desired result is to try to directly force the temperature field itself to be quasi-uniform. Thus, now, given a velocity field $\mathbf{u}$, we would seek a temperature field T and a control field g such that the functional

$$\mathcal{J}(T,g) = \frac{1}{2\gamma}\int_{\Gamma_O} |T - T_d|^2\, d\Gamma + \frac{\kappa\delta}{2}\int_{\Gamma_C} |g|^2\, d\Gamma \tag{1.10}$$

is minimized subject to (1.1)-(1.8), where T_d is some desired temperature distribution, *e.g.*, something close to the average temperature along Γ_C for the uncontrolled system. The non-negative parameters γ and δ can be used to change the relative importance of the the two terms appearing in the definition of $\mathcal{J}$ as well as to act as penalty parameters. As will be demonstrated by numerical examples in §6, a small γ is more useful in achieving quasi-uniform boundary temperature distributions, although it also reduces the accuracy of the

approximate solution. We will examine the latter issue in §4. Numerical experiments show that both (1.9) and (1.10) work effectively for the desired objective. We will focus our discussion on (1.10) thoroughout this paper.

Under the realistic assumption that $\mathbf{u} \cdot \mathbf{n} = 0$ on $\Gamma_C \cup \Gamma_N$, we may prove the existence and uniqueness of optimal solutions and derive an optimality system, *i.e.*, a set of equations from which the optimal control and state may be determined. Also, finite element methods are used to compute an approximate solution of the optimality system. Optimal error estimates are derived and numerical examples are presented. We have also developed an iterative algorithm to compute the approximate solution. The convergence of our algorithm is proved and a comparison with the direct method is made.

Control problems for the fully coupled problem as well as temperature matching for the entire extrudate will be addressed elsewhere.

We close this section by introducing some of the notation used in subsequent sections. Throughout, C will denote a positive constant whose meaning and value changes with context. Also, $H^s(\mathcal{D}), s \in \mathbf{R}$, denotes the standard Sobolev space of order s with respect to the set $\mathcal{D}$, where $\mathcal{D}$ is either the flow domain Ω, or its boundary Γ, or part of that boundary. Of course, $H^0(\mathcal{D}) = L^2(\mathcal{D})$. Dual spaces will be denoted by $(\cdot)^*$. Of particular interest will be the space

$$H^1_D(\Omega) = \{S \in H^1(\Omega) \quad : \quad S = 0 \quad \text{on } \Gamma_D\}.$$

Norms of functions belonging to $H^s(\Omega)$, $H^s(\Gamma)$ and $H^s(\Gamma_C)$ are denoted by $\|\cdot\|_s$, $\|\cdot\|_{s,\Gamma}$ and $\|\cdot\|_{s,\Gamma_C}$, respectively.

The inner product in $L^2(\Omega)$ is denoted by $(\cdot,\cdot)$, that in $L^2(\Gamma)$ by $(\cdot,\cdot)_\Gamma$, that in $L^2(\Gamma_O)$ by $(\cdot,\cdot)_{\Gamma_O}$, and that in $L^2(\Gamma_C)$ by $(\cdot,\cdot)_{\Gamma_C}$. Since, in general, we will use L^2-spaces as pivot spaces, these notation will also be employed to denote pairings between Sobolev spaces and their duals.

We will use the bilinear form

$$a(T,S) = \int_\Omega \operatorname{grad} T \cdot \operatorname{grad} S \, d\Omega \quad \forall\, T, S \in H^1(\Omega)$$

and the trilinear form

$$c(\mathbf{u},T,S) = \int_\Omega (\mathbf{u} \cdot \operatorname{grad} T)\, S \, d\Omega \quad \forall\, \mathbf{u} \in \mathbf{H}^1(\Omega) \quad \text{and} \quad \forall\, T, S \in H^1(\Omega).$$

These forms are continuous in the sense that there exist constants c_a and $c_c > 0$ such that

$$|a(T,S)| \le c_a \|T\|_1 \|S\|_1 \quad \forall\, T, S \in H^1(\Omega) \tag{1.11}$$

and

$$|c(\mathbf{u},T,S)| \le c_c \|\mathbf{u}\|_1 \|T\|_1 \|S\|_1 \quad \forall\, \mathbf{u} \in \mathbf{H}^1(\Omega) \quad \text{and} \quad \forall\, T, S \in H^1(\Omega). \tag{1.12}$$

Moreover, we have the coercivity property

$$a(T,T) \ge C_a \|T\|_1^2 \quad \forall\, T \in H^1_0(\Omega) \tag{1.13}$$

for some constant $C_a > 0$.

For details concerning the notation employed and the inequalities (1.11)-(1.13), one may consult, *e.g.*, [1] and [7].

2. The Optimization Problem, Existence of Solutions, And Optimality System

We begin by giving a precise statement of the optimization problem we consider. We will assume the domain Ω is a polygon in $\mathbf{R}^2$. We first recall that (1.1)-(1.4) uncouples from (1.5)-(1.8). We may solve for $(\mathbf{u}, p_\mathcal{T})$ from (1.1)-(1.4) once and for all and then plug them into (1.5)-(1.8). Thus the only state variable is T, *i.e.*, the temperature field, and the only boundary control variable is g. The state and control variables are constrained to satisfy the system (1.5)-(1.8), which we recast into the following weak form: find $T \in H^1_D(\Omega)$ such that

$$\kappa\, a(T,S) + c(\mathbf{u},T,S) = (Q,S) + \kappa\,(g,S)_{\Gamma_C} + \kappa\,(H_N,S)_{\Gamma_N} \quad \forall\, S \in H^1_D(\Omega)\,, \tag{2.1}$$

where we have introduced the simplifying notation

$$Q = \bar{Q} + 2\mu(\operatorname{grad}\mathbf{u} + \operatorname{grad}\mathbf{u}^T) : (\operatorname{grad}\mathbf{u} + \operatorname{grad}\mathbf{u}^T)\,.$$

Note that since we seek $T \in H^1_D(\Omega)$,

$$T = 0 \quad \text{on } \Gamma_D\,. \tag{2.2}$$

Throughout, we will assume that the given velocity field $\mathbf{u}$ is smooth and satisfies

$$\operatorname{div}\mathbf{u} = 0 \quad \text{in } \Omega \qquad \text{and} \qquad \mathbf{u}\cdot\mathbf{n} \geq 0 \quad \text{a.e. on } \Gamma_C \cup \Gamma_N\,. \tag{2.3}$$

Under these assumptions, we have the useful relation

$$c(\mathbf{u},S,S) = \frac{1}{2}\int_\Gamma (\mathbf{u}\cdot\mathbf{n})S^2\,d\Gamma \geq 0 \quad \forall\, S \in H^1(\Omega)\,, \tag{2.4}$$

which can be derived by setting $T = S$ in the following integration by parts formula:

$$c(\mathbf{u},T,S) = \int_\Gamma (\mathbf{u}\cdot\mathbf{n})TS\,d\Gamma - c(\mathbf{u},S,T)\,.$$

For each possible control function g, there exists a unique corresponding state function T.

Lemma 2.1– *For every $g \in L^2(\Gamma_C)$, there exists a unique $T \in H^1_D(\Omega)$ such that* (2.1) *is satisfied. Moreover,*

$$\|T\|_1 + \|T\|_{0,\Gamma_C} \leq C(\|g\|_{0,\Gamma_C} + \|Q\|_0 + \|H_N\|_{0,\Gamma_N})\,. \tag{2.5}$$ ∎

The *admissibility set* $\mathcal{U}_{ad}$ is defined by

$$\mathcal{U}_{ad} = \{(T,g) \in H^1_D(\Omega) \times L^2(\Gamma_C) : \mathcal{J}(T,g) < \infty, \text{ (2.1) is satisfied}\}\,. \tag{2.6}$$

Then, $(\hat{T},\hat{g}) \in \mathcal{U}_{ad}$ is called an *optimal solution* if there exists $\epsilon > 0$ such that

$$\mathcal{J}(\hat{T},\hat{g}) \leq \mathcal{J}(T,g) \quad \forall\,(T,g) \in \mathcal{U}_{ad} \text{ satisfying } \|T-\hat{T}\|_1 + \|g-\hat{g}\|_{0,\Gamma_c} \leq \epsilon\,. \tag{2.7}$$

Based on the previous lemma, we can show the existence and uniqueness of optimal solutions.

Theorem 2.2– *There exists a unique optimal solution $(\hat{T},\hat{g}) \in \mathcal{U}_{ad}$.* ∎

Using techniques in *e.g.* [9] we may obtain the optimality condition

$$g = -\frac{1}{\delta}\,\Phi|_{\Gamma_C} \tag{2.8}$$

where Φ is the solution of the adjoint state equation

$$\kappa\, a(R,\Phi) + c(\mathbf{u},R,\Phi) - \frac{1}{\gamma}(R, T - T_d)_{\Gamma_C} = 0 \quad \forall\, R \in H^1_D(\Omega)\,. \tag{2.9}$$

Eliminating g from (2.1) and combining with (2.9), we obtain the *optimality system*

$$\kappa\, a(T,S) + c(\mathbf{u},T,S) + \frac{\kappa}{\delta}(\Phi,S)_{\Gamma_C} = (Q,S) + \kappa\,(H_N,S)_{\Gamma_N} \quad \forall\, S \in H^1_D(\Omega) \tag{2.10}$$

and

$$\kappa\, a(R,\Phi) + c(\mathbf{u},R,\Phi) - \frac{1}{\gamma}(R, T - T_d)_{\Gamma_C} = 0 \quad \forall\, R \in H^1_D(\Omega)\,. \tag{2.11}$$

Thus, the optimal state, *i.e.*, the temperature distribution T, can be found by solving the coupled system (2.10)-(2.11), which also provides the optimal co-state Φ. The optimal control g can then be deduced from (2.8).

3. Finite Element Approximation, Error Estimates, and Iterative Methods

In the usual manner, one may construct finite element subspaces $W^h \subset H^1_D(\Omega) \cap C(\overline{\Omega})$ parametrized by a parameter h that tends to zero. (In practice, h is, of course, related to a grid size.) We assume the approximation property (see [3]): there exist an integer k and a constant C such that

$$\inf_{S^h \in W^h} \|S - S^h\|_1 \le C h^m \|S\|_{m+1} \quad \forall\, S \in H^1_D(\Omega) \text{ and } 0 \le m \le k\,. \tag{3.1}$$

A finite element algorithm for determining approximations of the solution of the optimality system (2.9)-(2.10) is then defined as follows: seek $T^h \in W^h$ and $\Phi^h \in W^h$ such that

$$\begin{aligned} \kappa\, a(T^h,S^h) + c(\mathbf{u},T^h,S^h) + \frac{\kappa}{\delta}(\Phi^h,S^h)_{\Gamma_C} \\ = (Q,S^h) + \kappa\,(H_N,S^h)_{\Gamma_N} \quad \forall\, S^h \in W^h \end{aligned} \tag{3.2}$$

and

$$\kappa\, a(R^h,\Phi^h) + c(\mathbf{u},R^h,\Phi^h) - \frac{1}{\gamma}\left(R^h, T^h - T_d\right)_{\Gamma_C} = 0 \quad \forall\, R^h \in W^h\,. \tag{3.3}$$

Although the optimality system is linear, the coupling of $\mathbf{u}$ and Φ in the two equations make the derivation of error estimates nontrivial. It turns out to be convenient to apply the *Brezzi-Rappaz-Raviart* theory (see [2], [5], and [7]) to obtain error estimates.

Theorem 3.1- *Let* (T,Φ) *and* (T^h,Φ^h) *be the solutions of* (2.9)-(2.10), *and* (3.2)-(3.3), *respectively. Assume that* T, $\Phi \in H^{m+1}(\Omega) \cap H^1_D(\Omega)$ *for some* $1 \le m \le k$; *also assume that* (3.1) *holds. Then,*

$$\begin{aligned} &\|T - T^h\|_1 + \|\Phi - \Phi^h\|_1 \\ &\quad \le C \max\left\{\frac{1}{\delta}, \frac{1}{\gamma}, 1\right\} h^m \left(\|Q\|_{m-1} + \|H_N\|_{\Gamma_N, m-1/2} + \|T_d\|_{\Gamma_C, m-1/2}\right), \end{aligned}$$

where C *is independent of* h, δ, γ, T, *and* Φ. ∎

A simple iterative algorithm for solving (2.10)-(2.11) can be defined as follows:

choose $\Phi^{(0)}$;

for $n = 1, 2, \ldots$, solve for $T^{(n)}$ from

$$\kappa\, a(T^{(n)}, S) + c(\mathbf{u}, T^{(n)}, S) = -\frac{\kappa}{\delta}(\Phi^{(n-1)}, S)_{\Gamma_C} + (Q, S) + \kappa\,(H_N, S)_{\Gamma_N} \quad \forall\, S \in H^1_D(\Omega)\,; \tag{3.4}$$

then solve for $\Phi^{(n)}$ from

$$\kappa\, a(R, \Phi^{(n)}) + c(\mathbf{u}, R, \Phi^{(n)}) = \frac{1}{\gamma}(R, T^{(n)} - T_d)_{\Gamma_C} \quad \forall\, R \in H^1_D(\Omega)\,. \tag{3.5}$$

Of course, ultimately, this algorithm has to be carried out in a discretized version, such as one using a finite element method.

The convergence of this algorithm can be proved as a result of the observation that it is effectively a gradient method for the following minimization problem: find $g \in L^2(\Gamma_C)$ such that $\mathcal{K}(g) := \mathcal{J}(T(g), g)$ is minimized where $T(g) \in H^1_D(\Omega)$ is defined as the solution of (2.1).

Theorem 5.2- *Let* $(T^{(n)}, \Phi^{(n)})$ *be the solution of* (3.4)-(3.5) *and* (T, Φ) *the solution of* (2.9)-(2.10). *Then,* $T^{(n)} \to T$ *in* $H^1_D(\Omega)$ *and* $\Phi^{(n)} \to \Phi$ *in* $H^1_D(\Omega)$ *as* $n \to \infty$. ∎

4. Computational Examples

Let $\Omega \subset \mathbb{R}^2$ be the unit square $(0,1) \times (0,1)$. Let $\Gamma = \Gamma_C \cup \Gamma_D \cup \Gamma_N \cup \Gamma_O$ be shown as in Figure 1.

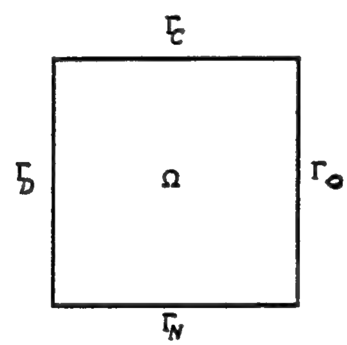

Figure 1. Computational domain

The finite element spaces W^h are chosen to be piecewise linear elements on a triangular mesh. All the numerical results make use of the following parameters and data:

parameters: $\kappa = 1/0.73\,; \quad Re = 1\,; \quad We = 1\,; \quad \omega = 1/2\,;$

boundary data: $T = 1 \quad \text{on } \Gamma_D\,, \qquad \dfrac{\partial T}{\partial n} = 0 \quad \text{on } \Gamma_N \cup \Gamma_O\,;$

heat source:

$$Q = -\frac{5\kappa}{2}\left(9\pi^2 \cos(3\pi x)\,\cos^2(\pi y) - 4\pi^2 \sin^2(\tfrac{3}{2}\pi x)\,\cos(2\pi y)\right) + (1 - y^2)\frac{15\pi}{2}\sin(3\pi x)\,\cos^2(\pi y)\,;$$

velocity profile: $\mathbf{u} = (1 - y^2, 0)\,,$

elastic extra stress profile: $\boldsymbol{\tau} = \begin{pmatrix} 0 & -y \\ -y & -4y^2 \end{pmatrix}\,,$

pressure profile: $p = 4(1 - y^2) - x\,.$

In functional (1.10), we choose

$$T_d = 3.5\,.$$

For the data given above, the exact solution of the uncontroled problem, *i.e.*, for

$$\frac{\partial T}{\partial n} = 0 \quad \text{on } \Gamma_C\,,$$

is given by $T = 5\,\sin^2(\frac{3}{2}\pi x)\,\cos^2(\pi y) + 1$.

We compare the temperature distribution in the uncontroled case with the optimal temperature distribution in the controled case for which

$$\frac{\partial T}{\partial n} = g \quad \text{on } \Gamma_C\,,$$

where g is the control such that (1.10) is minimized. Approximations to the optimal state and co-state are computed from (3.2)-(3.3); the approximate optimal control g^h is then obtained from (2.8), *i.e.*, $g^h = -(1/\delta)\Phi^h|_{\Gamma_C}$. All of the computational results shown below were obtained with the use of a mesh size $h = \frac{1}{19}$. Of course, calculations with varying mesh sizes were performed. Since these merely verified the error estimates, we do not report on them here.

Specifically, Figures 2-4 deal with the following cases:

1. Exact, uncontroled temperature and; Optimal temperature;
2. Exact, uncontroled temperature and; Optimal temperature;
2. Optimal boundary control.

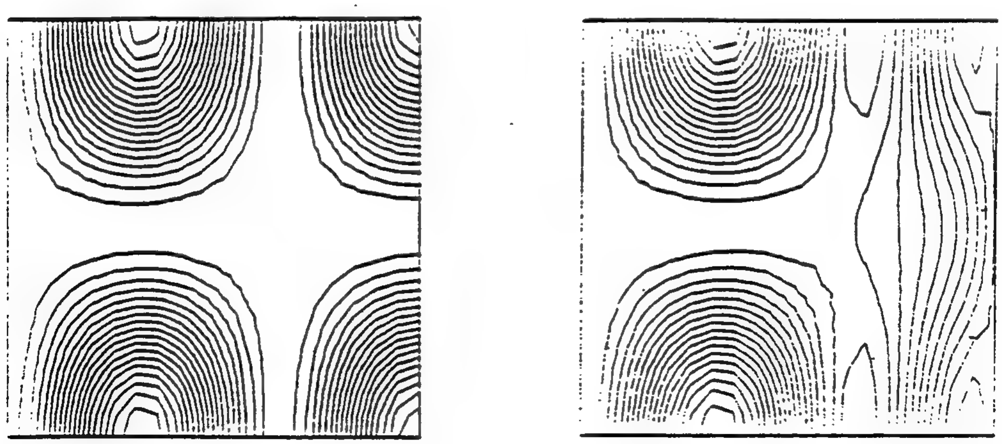

Figure 2. Temperature contours: uncontroled and controled.
Optimal boundary control on Γ_C.
(Γ_C is the top boundary segment.)
(Γ_O is the right boundary segment.)

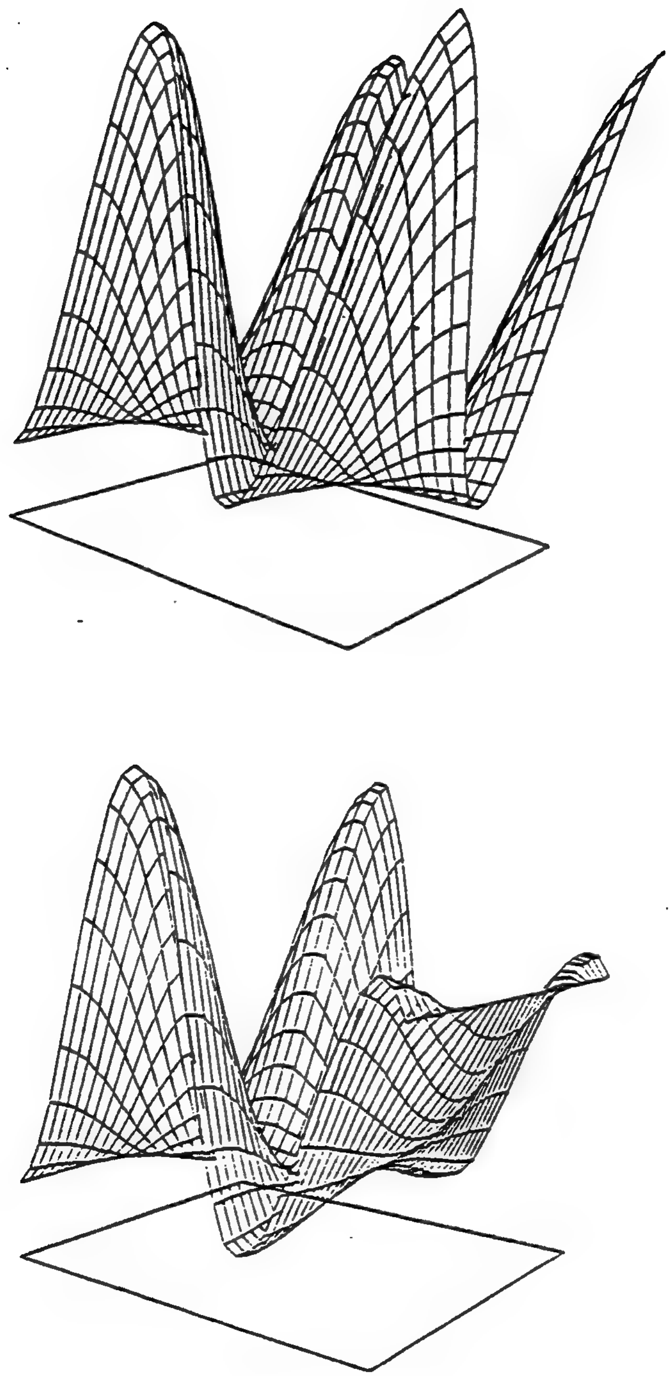

Figure 3. Temperature surfaces: uncontroled and controled.
(Γ_C is the top-right boundary segment.)
(Γ_O is the lower-right boundary segment.)

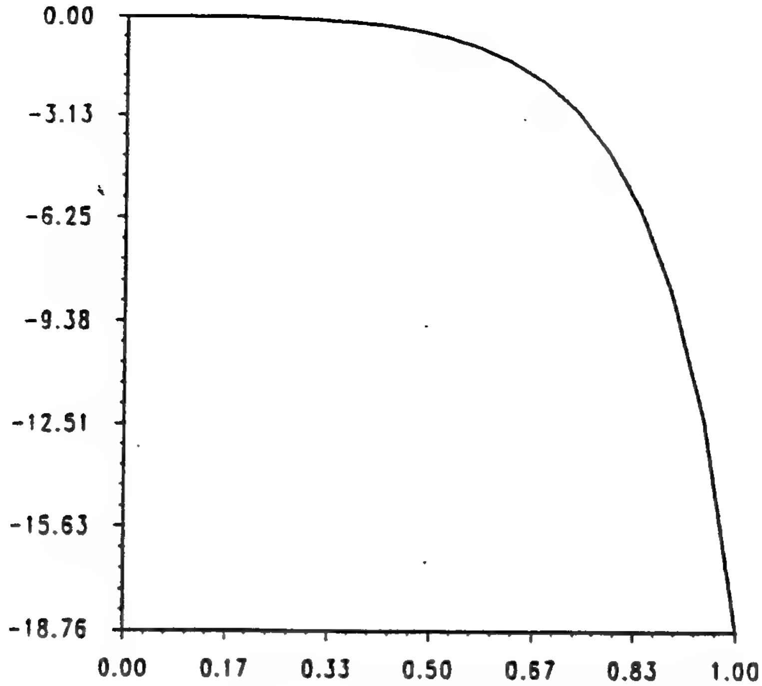

Figure 4. Optimal boundary control on Γ_C.

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ANALYSIS AND FINITE ELEMENT APPROXIMATION OF AN OPTIMAL CONTROL PROBLEM IN ELECTROCHEMISTRY WITH CURRENT DENSITY CONTROLS

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ABSTRACT. An optimal control problem for impressed cathodic systems in electrochemistry is studied. The control in this problem is the current density on the anode. A matching objective functional is considered; (many other objective functionals can be similarly treated.) The existence of an optimal solution is proved. The use of Lagrange multiplier rules is justified and an optimality system of equations is established. Finally, a finite element algorithm is defined and optimal error estimates are derived.

Key words. Optimal control, impressed cathodic system, electrochemistry, nonlinear boundary condition, finite element method, error estimate

AMS(MOS) subject classifications. 49J20, 49K20, 65K10, 65N15, 65N30

1. INTRODUCTION

We consider an optimal control problem for impressed cathodic systems. A typical example of an impressed cathodic system is a metal container filled with an electrolyte. The painted portion of the container surface is usually treated as insulated. The unpainted part is divided into cathode and anode which are connected to the negative and positive poles of an electrical source, respectively. By adjusting the current density on the anode we could effectively alter the potential distribution on the entire bounding surface or in the entire flow domain. The potential distribution, of course, has a direct effect on the chemical reaction process occurring inside the flow domain, which in turn has an effect on the rate of corrosion of the metal container. Thus the current density on the anode can be used as a practical control variable for generating a desired potential field. This idea can be conveniently formulated as optimal control problems for the potential equation with appropriate boundary conditions. Optimal control problems of this sort has been studied in [20] and [21] where the goal was to match a desired potential distribution

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on the cathode. The models analyzed in [20] and [21] are essentially linear. [14] discussed. mainly from an algorithmic point of view, several control mechanisms including adjusting the positions of anodes and/or the current density on the anodes in order to best match a desired potential on the structure surface; nonlinear models were employed as well as linear ones. [15] analyzed a "location control" problem, *i.e.*, the control variable is the location of anodes, wherein nonlinear models with boundary conditions of polynomial or mixed polynomial-exponential growth type were considered. In this article, we will attempt to mathematically analyze optimal control problems with current density controls. The nonlinear model used involves an exponentially growing boundary condition.

We assume the electrolyte occupies a physical domain $\Omega \in \mathbf{R}^2$ with a boundary Γ. The domain is assumed to be finite in this paper, although infinite domain problems can be handled if appropriate decay rate at infinity is assumed. If $\Omega \subset \mathbf{R}^3$, we will need to work with a non-Hilbert space $W^{1,p}(\Omega)$ with, *e.g.*, $p = 3$; similar results can still be obtained.

The electrical potential ϕ in Ω is governed by the differential equation

$$-\operatorname{div}(\sigma \operatorname{grad} \phi) = 0 \quad \text{in } \Omega,$$

where the conductivity σ is a continuous function with a positive lower bound.

The boundary Γ is divided into three components: the anode Γ_A, the cathode Γ_C and the insulated part Γ_0. On the cathode Γ_C, ϕ satisfies the relation

$$\sigma \frac{\partial \phi}{\partial n} = -f(\phi) \quad \text{on } \Gamma_C,$$

where f is an empirical function that depends on the electrode materials (see [4]). In particular we will assume f is given by the Butler-Volmer function:

$$f(\phi) = C_3[e^{C_1\phi} - e^{-C_2\phi}] \tag{1.1}$$

where C_1. C_2 and C_3 are positive constants (see [4]). Throughout this paper, f will be assumed to be defined by (1.1). For notational convenience, we will mainly use $f(\phi)$ rather than the explicit expression given in (1.1).

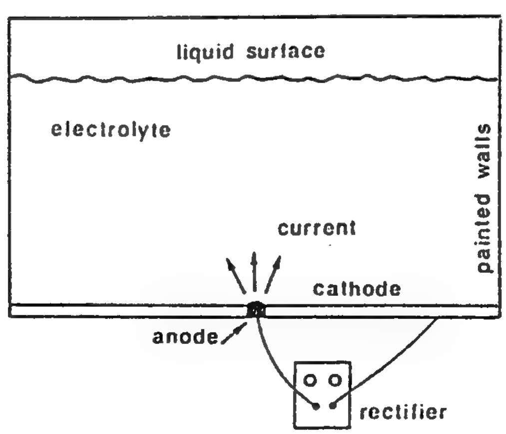

FIG. 1. **A typical impressed cathodic system: an electrolyte container connected with an electrical current source**

On the anode Γ_A, we have the boundary condition

$$\sigma \frac{\partial \phi}{\partial n} = u \quad \text{on } \Gamma_A \,,$$

which corresponds to the specification of the current density on the anode. Adjusting the current density on Γ_A amounts to treating u as a control variable. On the insulated part Γ_0,

$$\sigma \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \Gamma_0 \,.$$

We are concerned with the following optimal control problem: seek a state ϕ and a control u such that the functional

$$\mathcal{J}(\phi, u) = \frac{1}{2\epsilon_0} \int_\Omega (\phi - \phi_0)^2 \, d\Omega + \frac{\delta_0}{2} \int_{\Gamma_A} u^2 \, d\Gamma \,, \tag{1.2}$$

is minimized subject to the the constraint equations

$$-\operatorname{div}(\sigma \operatorname{grad} \phi) = 0 \quad \text{in } \Omega \tag{1.3}$$

$$\sigma \frac{\partial \phi}{\partial n} = u \quad \text{on } \Gamma_A \,, \tag{1.4}$$

$$\sigma \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \Gamma_0 \tag{1.5}$$

and

$$\sigma \frac{\partial \phi}{\partial n} = -f(\phi) \quad \text{on } \Gamma_C \,. \tag{1.6}$$

In (1.2) ϕ_0 is a desired potential distribution in Ω and ϵ_0 and δ_0 are positive constants.

We will make use of an equivalent variational formulation (1.7) of the nonlinear boundary value problem (1.3)-(1.6). We will utilize Sobolev spaces $H^m(\Omega)$, $H^s(\Gamma_A)$, $H^s(\Gamma_C)$. $H^s(\Gamma_0)$ and $H^s(\Gamma)$. The corresponding norms on these spaces will be denoted by, *e.g.*, $\|\cdot\|_m$, $\|\cdot\|_{s,\Gamma_A}$, etc. For details, see [1] and [8]. A weak formulation of (1.3)-(1.6) is given as follows: seek a $\phi \in H^1(\Omega)$ such that

$$\int_\Omega \sigma \operatorname{grad} \phi \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\phi) \psi \, d\Gamma = \int_{\Gamma_A} u \psi \, d\Gamma \,, \quad \forall \, \psi \in H^1(\Omega) \,. \tag{1.7}$$

Equation (1.7) can be formally shown to be equivalent to the nonlinear boundary value problem (1.3)-(1.6). We mention that second order elliptic differential equations with exponentially growing coefficients were studied in, among others, [9], [12]. [13] and [16]. An elliptic equation with mixed Dirichlet-Neumann type boundary conditions that have an exponentially growing coefficient in the boundary condition was studied [7]. Some of the techniques in these articles are useful for the mathematical and numerical analysis of the state equation (1.7).

We restate the minimization problem as follows:

$$\begin{array}{l} \text{seek a state } \phi \in H^1(\Omega) \text{ and a } u \in U \text{ such that the} \\ \text{functional (1.2) is minimized subject to (1.7),} \end{array} \tag{1.8}$$

where

$$U \text{ is a non-empty, closed, convex subset of } L^2(\Gamma_A). \tag{1.9}$$

Now we state a few useful facts. We set $\alpha = \frac{1}{2}C_3 \min\{C_1, C_2\}$. Then by Mean Value Theorem we obtain

$$f(\phi)\phi = C_3(C_1 + C_2)\, e^{\tilde{\phi}} \phi^2 \geq 2\alpha\phi^2 \quad \forall\, \phi \tag{1.10}$$

where $\tilde{o}$ is between $(C_1\phi)$ and $(-C_2\phi)$. It is also easy to see that

$$f'(\phi) \geq 2\alpha \quad \forall\, \phi\,. \tag{1.11}$$

The norm on $H^1(\Omega)$ defined by

$$|||\phi|||_1 = \left\{ \int_\Omega \sigma |\operatorname{grad}\phi|^2\, d\Omega + 2\alpha \int_{\Gamma_C} \phi^2\, d\Gamma \right\}^{1/2} \quad \forall\, \phi \in H^1(\Omega)$$

is equivalent to the usual $H^1(\Omega)$-norm $\|\cdot\|_1$, *i.e.*,there exist constants $\rho > 0$ and $\gamma > 0$ such that

$$\rho\, \|o\|_1^2 \geq \int_\Omega \sigma |\operatorname{grad}\phi|^2\, d\Omega + 2\alpha \int_{\Gamma_C} \phi^2\, d\Gamma \geq \gamma\, \|\phi\|_1^2 \quad \forall\, \phi \in H^1(\Omega)\,. \tag{1.12}$$

A proof of (1.12) can found in, *e.g.*, [17].

The rest of the paper is organized as follows. In §2 we prove the existence and uniqueness of solutions to (1.7) so that the constraint equation is well-posed. In §3 we show the existence of an optimal pair $(\hat{\phi}, \hat{u})$ that minimizes (1.1) subject to (1.7). In §4 we justify the use of Lagrange multiplier rules and derive an optimality condition. In §5 we discuss the regularity of optimal solutions. Finally in §6 we define a finite element algorithm for solving the optimality system and derive optimal error estimates.

2. Existence and Uniqueness of Solutions to the Constraint Equations

We first examine the existence of a solution to the nonlinear Neumann type boundary value problems (1.7).

Lemma 2.1 *X be a finite-dimensional Hilbert space whose scalar product is denoted by $(\cdot,\cdot)$ and the corresponding norm by $|\cdot|$. Let F be a continuous mapping form X into X with the following property: there exists an $r > 0$ such that*

$$(F(\phi), \phi) \geq 0 \quad \forall\, \phi \in X \text{ with } |\phi| = r\,.$$

Then there exists an $\phi \in X$ such that

$$F(\phi) = 0 \quad \text{and} \quad |\phi| \leq r\,.$$

Proof. See [Raviart], pp. 279. ∎

Lemma 2.2 *Assume $\phi \in H^1(\Omega)$ and $s > 0$. Then $e^{s|\phi|} \in L^1(\Gamma)$. Moreover, there exists a constant κ, independent of ϕ, such that*

$$\int_\Gamma e^{s|\phi|}\, d\Gamma \leq 1 + |\Gamma| + e^{s^2\kappa^2\|\phi\|_1^2}\, |\Gamma| < \infty\,,$$

where $|\Gamma|$ is the measure of Γ.

Proof. Let $\phi \in H^1(\Omega)$ and $s > 0$ be given. A Sobolev embedding theorem implies $\phi \in H^{1/2}(\Gamma)$. Using embedding results for Orlicz-Sobolev spaces (see [1], [10] and [18]) (recall $\Omega \subset \mathbf{R}^2$), we have $H^{1/2}(\Gamma) \hookrightarrow L_A(\Gamma)$ where the N-function $A(t) = e^{t^2} - 1$. Thus there exists a constant $\kappa > 0$ such that

$$\|\phi\|_{L_A(\Gamma)} \equiv \inf \left\{ k : \int_\Gamma e^{\frac{|\phi|^2}{k^2}}\, d\Gamma \leq 1 \right\} \leq \kappa \|\phi\|_1 < \infty\,.$$

Hence for each sufficiently $\epsilon > 0$, the constant $k \equiv \|\phi\|_{L_A(\Gamma)} + \epsilon$ satisfies

$$\int_\Gamma [e^{\frac{|\phi|^2}{k^2}} - 1]\, d\Gamma \leq 1 \quad \text{so that} \quad \int_\Gamma e^{\frac{|\phi|^2}{k^2}}\, d\Gamma \leq 1 + |\Gamma|\,.$$

We set $M = sk^2$. By an elementary calculation we can show that

$$e^{sx} < e^{\frac{x^2}{k^2}} \quad \forall\, |x| > M\,.$$

We set $K = e^{sM} = e^{s^2k^2} < \infty$. Then

$$\begin{aligned}
\int_\Gamma e^{s|\phi|}\, d\Gamma &= \int_{\{\mathbf{x}\in\Gamma : |\phi(\mathbf{x})| \geq M\}} e^{s|\phi|}\, d\Gamma + \int_{\{\mathbf{x}\in\Gamma : |\phi(\mathbf{x})| < M\}} e^{s|\phi|}\, d\Gamma \\
&\leq \int_\Gamma e^{\frac{|\phi|^2}{k^2}}\, d\Gamma + K\,|\Gamma| \leq 1 + |\Gamma| + e^{s^2(\|\phi\|_{L_A(\Gamma)}+\epsilon)^2}\, |\Gamma| \\
&\leq 1 + |\Gamma| + e^{s^2(\kappa\|\phi\|_1+\epsilon)^2}\, |\Gamma| < \infty\,.
\end{aligned}$$

Letting $\epsilon \to 0$ yield the desired result. ∎

Lemma 2.3 *Assume $\{\phi_n\} \subset L^2(\Gamma_C)$ is a sequence such that $\phi_n \to \phi$ a.e. on Γ_C and*

$$\int_{\Gamma_C} f(\phi_n)\phi_n\, d\Gamma \leq B \quad \forall\, n \tag{2.1}$$

where f is defined by (1.1) and $B > 0$ is a constant independent of n. Then

$$\int_{\Gamma_C} f(\phi)\phi\, d\Gamma \leq \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n\, d\Gamma$$

and

$$\lim_{n\to\infty} \int_{\Gamma_C} |f(\phi_n) - f(\phi)|\, d\Gamma = 0\,.$$

Proof. The proof follows the ideas of [13], pp. 21-22. Since f is continuous and $\phi_n \to o$ a.e. on Γ_C, we deduce that $f(\phi_n) \to f(\phi)$ a.e. on Γ_C. Note that $f(\phi)\phi \geq 0$ on Γ_C so that we may use Fatou's Lemma to obtain

$$\int_{\Gamma_C} f(\phi)\phi \, d\Gamma \leq \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma \leq B .$$

Hence $f(\phi)\phi \in L^1(\Omega)$. By setting $K = \sup_{|x|\leq 1} |f(x)|$ we easily conclude from the identity

$$|f(t)| = |t|^{-1} f(t)t \quad \forall\, t \neq 0 \tag{2.2}$$

that

$$|f(t)| \leq f(t)t + K \quad \forall\, t \in \mathbf{R} .$$

Thus

$$|f(\phi)| \leq |f(\phi)|\,|\phi| + K \quad \text{on } \Gamma_C ,$$

i.e., $f(o) \in L^1(\Gamma_C)$. Utilizing (2.2) again, we deduce that for each $\delta > 0$ and for a.e. $\mathbf{x} \in \Gamma_C$, we have either

$$|\phi_n| \leq \delta^{-1} \quad \text{or} \quad |f(\phi)| \leq \delta f(\phi_n)\,\phi_n$$

so that

$$|f(\phi)| \leq C_\delta + \delta f(\phi_n)\,\phi_n \quad \text{on } \Gamma_C ,$$

where $C_\delta = \sup\limits_{|x|\leq \delta^{-1}} |f(x)|$. For every measurable subset $S \subset \Gamma_C$ we have

$$\int_{\Gamma_C} |f(\phi_n)|\, d\Gamma \leq C_\delta |S| + \delta \int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma .$$

Equation (2.1) implies

$$\int_S f(\phi_n)\phi_n \, d\Gamma \leq 2B$$

for n greater than some $N_0 > 0$. Thus

$$\int_S |f(\phi_n)|\, d\Gamma \leq C_\delta |S| + 2B\delta \quad \forall\, n > N_0 ,$$

where $|S|$ is the measure of S. Hence, the sequence of functions $\{f(\phi_n)\}$ has equi-absolutely continuous integrals. By Vitali's Convergence Theorem,

$$\lim_{n\to\infty} \int_{\Gamma_C} |f(\phi_n) - f(\phi)|\, d\Gamma = 0 . \quad \blacksquare$$

Theorem 2.4 *Assume $u \in L^2(\Gamma_A)$. Then there exists a unique $\phi \in H^1(\Omega)$ that satisfies* (1.7). *Furthermore, ϕ satisfies the estimate*

$$\|\phi\|_1 \leq \frac{\beta}{\gamma} \{\|u\|_{0,\Gamma_A} + 1\} , \tag{2.3}$$

where β and γ are constants independent of ϕ.

Proof. We first establish an inequality

$$\int_\Omega \sigma \operatorname{grad}\phi \cdot \operatorname{grad}\phi \, d\Omega + \int_{\Gamma_C} f(\phi)\phi \, d\Gamma - \int_{\Gamma_A} u\phi \, d\Gamma \geq$$
$$\geq 0 \quad \forall\, \phi \in H^1(\Omega) \text{ with } \|\phi\|_1 = r$$

for some $r > 0$. Using (1.10) we have that

$$\int_{\Gamma_C} f(\phi)\phi \, d\Gamma \geq \alpha \int_{\Gamma_C} \phi^2 \, d\Gamma \quad \forall\, \phi \in H^1(\Omega).$$

Hence it follows from (1.12) that

$$\int_\Omega \sigma \operatorname{grad}\phi \cdot \operatorname{grad}\phi \, d\Omega + \int_{\Gamma_C} f(\phi)\phi \, d\Gamma \geq \gamma\|\phi\|_1^2 \quad \forall\, \phi \in H^1(\Omega).$$

Using Cauchy-Schwartz inequality and trace theorems we obtain the estimate

$$\left|\int_{\Gamma_A} u\phi \, d\Gamma\right| \leq \beta\|\phi\|_1\|u\|_{0,\Gamma_A} \quad \forall\, \phi \in H^1(\Omega),$$

where β is a positive constant. By combining the last two estimates we deduce that for $r = \frac{\beta}{\gamma}\{\|u\|_{0,\Gamma_A} + 1\} > 0$ we have

$$\int_\Omega \sigma \operatorname{grad}\phi \cdot \operatorname{grad}\phi \, d\Omega + \int_{\Gamma_C} f(\phi)\phi \, d\Gamma - \int_{\Gamma_A} u\phi \, d\Gamma \geq$$
$$\geq 0 \quad \forall\, \phi \in H^1(\Omega) \text{ with } \|\phi\|_1 = r. \tag{2.4}$$

Since $H^1(\Omega)$ is separable, we may choose a countable basis of $H^1(\Omega)$: $\{\psi_i\}_{i=1}^\infty$. We set $X_n = \operatorname{span}\{\psi_1, \cdots, \psi_n\}$. The inner product and norm on each X_n is defined by that of $H^1(\Omega)$ restricted to X_n. We introduce the mapping $F_n : X_n \to X_n$ as follows. For each $\phi \in H^1(\Omega)$, $F_n(\phi) \in X_n$ is defined by

$$(F_n(\phi), \psi_j) = \int_\Omega \sigma \operatorname{grad}\phi \cdot \operatorname{grad}\psi_j \, d\Omega + \int_{\Gamma_C} f(\phi)\psi_j \, d\Gamma - \int_{\Gamma_A} u\psi_j \, d\Gamma \quad 1 \leq j \leq n.$$

It follows from (2.4) and Lemma 2.1 that the finite dimensional problem

$$\int_\Omega \operatorname{grad}\phi_n \cdot \operatorname{grad}\psi \, d\Omega + \int_{\Gamma_C} f(\phi_n)\psi \, d\Gamma = \int_{\Gamma_A} u\psi \, d\Gamma, \quad \forall\, \psi \in X_n \tag{2.5}$$

has a solution $\phi_n \in X_n$ with a bound

$$\|\phi_n\|_1 \leq \frac{\beta}{\gamma}\{\|u\|_{0,\Gamma_A} + 1\}. \tag{2.6}$$

We can extract a subsequence of $\{\phi_n\}$, still denoted by $\{\phi_n\}$, that converges weakly to some $\phi \in H^1(\Omega)$ as $n \to 0$. Then $\{\phi_n\}$ also converges weakly in $H^{1/2}(\Gamma)$ by a trace theorem. Thus $\{\phi_n\}$ converges strongly in $L^2(\Gamma)$ by compact imbedding. This in turn implies a subsequence satisfies $\phi_n \to \phi$ a.e. on Γ. By setting $\psi = \phi_n$ in (2.5) we obtain

$$\int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma \le \|u\|_{0,\Gamma_A} \|\phi_n\|_{0,\Gamma_A}$$
$$\le C\|u\|_{0,\Gamma_A} \|\phi_n\|_1 \le C \|u\|_{0,\Gamma_A} \frac{\beta}{\gamma} \{\|u\|_{0,\Gamma_A} + 1\} .$$

By Lemma 2.3 we have that

$$\int_{\Gamma_C} f(\phi)\phi \, d\Gamma \le \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n \, d\Gamma$$

and

$$\lim_{n\to\infty} \int_{\Gamma_C} |f(\phi_n) - f(\phi)| \, d\Gamma = 0 .$$

By passing to the limit in (2.5) for each $\psi \in C^\infty(\overline{\Omega})$ we see that

$$\int_\Omega \sigma \,\mathrm{grad}\, \phi \cdot \mathrm{grad}\, \psi \, d\Omega + \int_{\Gamma_C} f(\phi)\psi \, d\Gamma = \int_{\Gamma_A} u\psi \, d\Gamma , \quad \forall\, \psi \in C^\infty(\overline{\Omega}) . \tag{2.7}$$

We next prove that this ϕ is a solution to (1.7). For each $\psi \in H^1(\Omega)$, we may choose a sequence $\{\psi_k\} \subset C^\infty(\overline{\Omega})$ such that $\|\psi - \psi_k\|_1 \to 0$ as $k \to \infty$. Using (2.7) we have

$$\int_\Omega \sigma \,\mathrm{grad}\, \phi \cdot \mathrm{grad}\, \psi_k \, d\Omega + \int_{\Gamma_C} f(\phi)\psi_k \, d\Gamma = \int_{\Gamma_A} u\psi_k \, d\Gamma , \quad \forall\, k . \tag{2.8}$$

Lemma 2.2 implies $e^{C_1\phi} \in L^2(\Gamma_C)$ and $e^{-C_2\phi} \in L^2(\Gamma_C)$ so that $\int_{\Gamma_C} |f(\phi)|^2 \, d\Gamma < \infty$. Hence,

$$\left| \int_{\Gamma_C} f(\phi)(\psi - \psi_k) \, d\Gamma \right| \le \|f(\phi)\|_{0,\Gamma_C} \|\psi - \psi_k\|_{0,\Gamma_C} \le C\|f(\phi)\|_{0,\Gamma_C} \|\psi - \psi_k\|_1$$

so that

$$\int_{\Gamma_C} f(\phi)(\psi - \psi_k) \, d\Gamma \to 0 \quad \text{as } k \to \infty .$$

Thus we may pass to the limit in (2.7) to show (1.7) holds. The estimate (2.3) follows easily from (2.6).

To answer the question of uniqueness, we assume ϕ and $\bar{\phi}$ are two solutions to (1.7). Then we have

$$\int_\Omega \sigma \,\mathrm{grad}(\phi - \bar{\phi}) \cdot \mathrm{grad}\, \psi \, d\Omega + \int_{\Gamma_C} [f(\phi) - f(\bar{\phi})]\psi \, d\Gamma = 0 , \quad \forall\, \psi \in H^1(\Omega) .$$

Setting $v = \phi - \bar{\phi}$, we see that

$$\int_\Omega \sigma |\operatorname{grad}(\phi - \bar{\phi})|^2 \, d\Omega + \int_{\Gamma_C} [f(\phi) - f(\bar{\phi})](\phi - \bar{\phi}) \, d\Gamma = 0 \, .$$

Using Mean Value Theorem,

$$\int_\Omega \sigma |\operatorname{grad}(\phi - \bar{\phi})|^2 \, d\Omega + \int_{\Gamma_C} f'(\tilde{\phi})(\phi - \bar{\phi})^2 \, d\Gamma = 0$$

for some $\tilde{\phi}$ between ϕ and $\bar{\phi}$. Using (1.11), we see that

$$\int_\Omega \sigma |\operatorname{grad}(\phi - \bar{\phi})|^2 \, d\Omega + \alpha \int_{\Gamma_C} (\phi - \bar{\phi})^2 \, d\Gamma \leq 0 \, .$$

Hence we deduce that $\operatorname{grad}(\phi - \bar{\phi}) = 0$ in Ω and $(\phi - \bar{\phi}) = 0$ on Γ_C. This in turn implies $(\phi - \bar{\phi}) = 0$ in Ω, *i.e.*, uniqueness holds. ∎

3. Existence of An Optimal Solution

Having shown that the constraint equation (1.7) is well-posed, we are now prepared to study the existence of an optimal solution $(\hat{\phi}, \hat{u})$ that minimizes the functional (1.2) subject to (1.7). We introduce the admissible set

$$\mathcal{U}_{ad} = \{(\phi, u) \in H^1(\Omega) \times U : (\phi, u) \text{ satisfies } (1.7)\} \, ,$$

where U is given by (1.9).

Theorem 3.1 *There exists a $(\hat{\phi}, \hat{u}) \in H^1(\Omega) \times U$ that minimizes* (1.2) *subject to* (1.7).

Proof. Theorem 2.4 implies an element $(\phi, u) \in \mathcal{U}_{ad}$ exists such that $\mathcal{J}(\phi, u) < \infty$. Let $\{(\phi_n, u_n)\} \subset \mathcal{U}_{ad}$ be a minimizing sequence, *i.e.*,

$$\lim_{n \to \infty} \mathcal{J}(\phi_n, u_n) = \inf_{(\phi, u) \in \mathcal{U}_{ad}} \mathcal{J}(\phi, u) \tag{3.1}$$

and

$$\int_\Omega \sigma \operatorname{grad} \phi_n \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\phi_n) \psi \, d\Gamma = \int_{\Gamma_A} u_n \psi \, d\Gamma \, , \quad \forall \, \psi \in H^1(\Omega) \, . \tag{3.2}$$

Using (1.2) and (3.1) we deduce $\{u_n\}$ is bounded in $L^2(\Gamma_A)$. Then (2.3) implies $\{\|\phi_n\|_1\}$ is bounded. Hence we may extract a subsequence $\{(\phi_n, u_n)\}$ such that

$$\phi_n \rightharpoonup \hat{\phi} \quad \text{in } H^1(\Omega) \qquad \text{and} \qquad u_n \rightharpoonup \hat{u} \quad \text{in } L^2(\Gamma_A) \, .$$

Furthermore, trace theorems implies $\phi_n \to \phi$ in $L^2(\Gamma_C)$; this in turn implies $\phi_n \to \phi$ a.e. on Γ_C (after extracting subsequences if necessary). By setting $\psi = \phi_n$ in (3.2) we obtain

$$\int_\Omega \sigma |\operatorname{grad} \phi_n|^2 \, d\Omega + \int_{\Gamma_C} f(\phi_n) \phi_n \leq \|u_n\|_{0,\Gamma_A} \|\phi_n\|_{0,\Gamma_A} \leq \beta \, \|u_n\|_{0,\Gamma_A} \|\phi_n\|_1 \, .$$

Hence we deduce

$$\int_{\Gamma_C} f(\phi_n)\phi_n \le M$$

where M is a constant independent of n. By Lemma 2.3,

$$\int_{\Gamma_C} f(\hat{\phi})\hat{\phi}\, d\Gamma \le \liminf_{n\to\infty} \int_{\Gamma_C} f(\phi_n)\phi_n\, d\Gamma$$

and

$$\lim_{n\to\infty} \int_{\Gamma_C} |f(\phi_n) - f(\hat{\phi})|\, d\Gamma = 0.$$

By passing to the limit in (3.2) for $\psi \in C^\infty(\overline{\Omega})$ we obtain

$$\int_\Omega \sigma \operatorname{grad} \hat{\phi} \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\hat{\phi})\psi\, d\Gamma = \int_{\Gamma_A} \hat{u}\psi\, d\Gamma\,, \quad \forall\, \psi \in C^\infty(\overline{\Omega})\,.$$

Then using the denseness of $C^\infty(\overline{\Omega})$ in $H^1(\Omega)$ and the fact that $f(\hat{\phi}) \in L^2(\Gamma_C)$, we obtain

$$\int_\Omega \sigma \operatorname{grad} \hat{\phi} \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f(\hat{\phi})\psi\, d\Gamma = \int_{\Gamma_A} \hat{u}\psi\, d\Gamma\,, \quad \forall\, \psi \in H^1(\Omega)\,.$$

Thus $(\hat{\phi}, \hat{u}) \in \mathcal{U}_{ad}$. Finally using the weak lower semi-continuity of $\mathcal{J}(\cdot,\cdot)$, we conclude that $(\hat{\phi}, \hat{u})$ is indeed an optimal solution, *i.e.*,

$$\mathcal{J}(\hat{\phi}, \hat{u}) = \inf_{(\phi,u)\in\mathcal{U}_{ad}} \mathcal{J}(\phi, u)\,. \quad \blacksquare$$

4. Lagrange Multiplier Rules

In this section we will attempt to characterize optimal solutions whose existence has been established in §3. Since the constraint equation has a unique solution for each given control u, the state ϕ is a well-defined function of u. Since U given in (1.9) is not necessarily an open set, the mapping $u \mapsto \phi$ is in general not differentiable. Although other approaches available, it turns out to be convenient to use the Lagrange multiplier rule to turn the constrained minimization problem (1.8) into an unconstrained one and derive an optimality condition.

We first quote the following abstract theorem concerning the existence of Lagrange multipliers for minimization problems on Banach spaces (see, *e.g.*, [19]):

Lemma 4.1. *Let B_1 and B_2 be two Banach spaces, and U an arbitrary set. Suppose $\mathcal{J}$ is a functional on $B_1 \times U$, $\mathcal{K}$ a mapping from $B_1 \times U$ to B_2. Assume $(\hat{\phi}, \hat{u}) \in B_1 \times U$ is a local minimum for the constrained minimization problem:*

$$\min \mathcal{J}(\phi, u) \quad \text{subject to} \quad \mathcal{K}(\phi, u) = 0\,, \tag{4.1}$$

i.e., there exists an open neighborhood Θ of $\hat{\phi}$ in B_1 such that

$$\mathcal{J}(\hat{\phi}, \hat{u}) \le \mathcal{J}(\phi, u) \quad \forall\, (\phi, u) \in \Theta \times U \text{ satisfying } \mathcal{K}(\phi, u) = 0\,.$$

Assume further the following conditions are satisfied:

(A) *for each $u \in U$, $\phi \mapsto \mathcal{J}(\phi, u)$ and $\phi \mapsto \mathcal{K}(\phi, u)$ are Frechet-differentiable in Θ:*

(B) *for every $\phi \in \Theta$, $u_1, u_2 \in U$ and $\alpha \in [0,1]$, there exists a $u_\alpha = u_\alpha(\phi, u_1, u_2) \in U$ such that*

$$\mathcal{K}(\phi, u_\alpha) = \alpha\mathcal{K}(\phi, u_1) + (1-\alpha)\mathcal{K}(\phi, u_2)$$

and

$$\mathcal{J}(\phi, u_\alpha) \le \alpha\mathcal{J}(\phi, u_1) + (1-\alpha)\mathcal{J}(\phi, u_2);$$

(C) *the algebraic sum of $\mathcal{K}_\phi(\hat{\phi}, \hat{u})B_1 + \mathcal{K}(\hat{\phi}, U)$ contains a neighborhood of 0.*

Then there exists a $\lambda \in B_2^*$ such that

$$\langle \mathcal{J}_\phi(\hat{\phi}, \hat{u}), \psi\rangle - \langle \lambda, \mathcal{K}_\phi(\hat{\phi}, \hat{u})\psi\rangle = 0 \quad \forall\, \psi \in B_1$$

and

$$\min_{u \in U} \mathcal{L}(\hat{\phi}, u, \lambda) = \mathcal{L}(\hat{\phi}, \hat{u}, \lambda),$$

where $\mathcal{L}(\phi, u, \lambda) \equiv \mathcal{J}(\phi, u) - \langle \lambda, \mathcal{K}(\phi, u)\rangle$ is the Lagrangian of the constrained minimization problem (4.1).

Proof: See [19]. ∎

We will fit our optimization problem (1.8) into the above abstract framework. We define the Banach spaces $B_1 \equiv H^1(\Omega)$ and $B_2 \equiv H^1(\Omega)^*$. Let U be given by (1.9). The (generalized) nonlinear constraint $\mathcal{K} : B_1 \times U \to B_2$ is defined as follows: $\mathcal{K}(\bar{\phi}, \bar{u}) = \bar{l}$ for $(\bar{\phi}, \bar{u}) \in B_1 \times U$ and $\bar{l} \in B_2$ if and only if

$$\begin{aligned}\langle \bar{l}, \psi\rangle_{\Gamma_A} = \int_\Omega \sigma \operatorname{grad}\bar{\phi} \cdot \operatorname{grad}\psi \, d\Omega + \int_{\Gamma_C} f(\bar{\phi})\psi \, d\Gamma& \\ - \int_{\Gamma_A} \bar{u}\psi \, d\Gamma \quad \forall\, \psi \in H^1(\Omega)&.\end{aligned} \tag{4.2}$$

We easily see that (1.8) is equivalent to

$$\begin{aligned}&\text{find } (\phi, u) \in B_1 \times U \text{ such that}\\ &\mathcal{J}(\phi, u) = \inf\left\{\mathcal{J}(\bar{\phi}, \bar{u}) : (\bar{\phi}, \bar{u}) \in B_1 \times U,\ \mathcal{K}(\bar{\phi}, \bar{u}) = 0\right\}.\end{aligned}$$

Let the Frechet derivative of $\mathcal{J}$ and $\mathcal{K}$ with respect to ϕ be denoted by $D_\phi\mathcal{J}$ and $D_\phi\mathcal{K}$, respectively. Let the Frechet derivative of $\mathcal{J}$ and $\mathcal{K}$ with respect to u be denoted by $D_u\mathcal{J}$ and $D_u\mathcal{K}$, respectively. $D_\phi\mathcal{K}(\phi, u) \in \mathcal{L}(B_1, B_2)$ is defined as follows. $D_\phi\mathcal{K}(\hat{\phi}, \hat{u}) \cdot \bar{\phi} = \bar{l}$ for $\bar{\phi} \in B_1$ and $\bar{l} \in B_2$ if and only if

$$\langle \bar{l}, \psi\rangle_{\Gamma_A} = \int_\Omega \sigma \operatorname{grad}\bar{\phi} \cdot \operatorname{grad}\psi \, d\Omega + \int_{\Gamma_C} f'(\phi)\bar{\phi}\psi \, d\Gamma \quad \forall\, \psi \in H^1(\Omega). \tag{4.3}$$

In order to apply Lemma 4.1, we need to verify conditions (A)–(C). We begin with the verification of (C).

Lemma 4.2. *Assume $(\hat{\phi}, \hat{u}) \in \mathcal{U}_{ad}$ is an optimal solution to* (1.7). *Then the operator $D_\phi \mathcal{K}(\hat{\phi}, \hat{u})$ is onto from B_1 to B_2.*

Proof: Using (1.11)-(1.12) we easily obtain the coercivity for the bilinear form

$$(\bar{\phi}, \psi) \mapsto \int_\Omega \sigma \operatorname{grad} \bar{\phi} \cdot \operatorname{grad} \psi \, d\Omega + \int_{\Gamma_C} f'(\phi) \bar{\phi} \psi \, d\Gamma \quad \forall \, \bar{\phi}, \; \psi \in H^1(\Omega).$$

Then Lax-Milgram Lemma implies that for any $\bar{l} \in H^1(\Omega)^*$ there exists a unique $\bar{\phi} \in H^1(\Omega)$ that solves (4.3). ∎

Now we are prepared to derive an optimality condition.

Theorem 4.3. *Assume $(\hat{\phi}, \hat{u}) \in \mathcal{U}_{ad}$ is an optimal solution to the minimization problem* (1.8). *Then there exists a $\lambda \in H^1(\Omega)$ such that*

$$\int_\Omega \sigma \operatorname{grad} \psi \cdot \operatorname{grad} \lambda \, d\Omega + \int_{\Gamma_C} f'(\hat{\phi}) \, \psi \lambda \, d\Gamma = \frac{1}{\epsilon_0} \int_\Omega (\hat{\phi} - \phi_0) \psi \, d\Omega \quad \forall \, \psi \in H^1(\Omega). \tag{4.4}$$

and

$$\int_{\Gamma_A} (\delta_0 \hat{u} + \lambda)(u - \hat{u}) \, d\Gamma \geq 0 \quad \forall \, u \in U. \tag{4.5}$$

Proof: Condition (A) in Lemma 4.1 is obviously satisfied for the present setting. The convexity in u for the constraint is readily verified since the control variable u enters the constraint equation in a linear manner and the control set U is convex. The convexity in u for the functional is also easily seen from the convexity of the mapping $u \mapsto \|u\|^2_{0,\Gamma_C}$. Thus Condition (B) is verified. The validity of Condition (C) is established in Lemma 4.2. Hence, by Lemma 4.1, there exists a $\lambda \in B_2^* = H^1(\Omega)$ that satisfies

$$\langle D_\phi \mathcal{J}(\hat{\phi}, \hat{u}), \psi \rangle - \langle \lambda, D_\phi \mathcal{K}(\hat{\phi}, \hat{u}) \cdot \psi \rangle = 0 \quad \forall \, \psi \in H^1(\Omega) \tag{4.6}$$

and

$$\min_{u \in U} \mathcal{L}(\hat{\phi}, u, \lambda) = \mathcal{L}(\hat{\phi}, \hat{u}, \lambda), \tag{4.7}$$

where

$$\mathcal{L}(\phi, u. \lambda) \equiv \mathcal{J}(\phi, u) - \left[\int_\Omega \sigma \operatorname{grad} \phi \cdot \operatorname{grad} \lambda \, d\Omega + \int_{\Gamma_C} f(\phi) \lambda \, d\Gamma - \int_{\Gamma_A} u \, \lambda \, d\Gamma \right]. \tag{4.8}$$

Using (1.2) and (4.3), which are the defining equations for $\mathcal{J}(\phi, u)$ and $D_\phi \mathcal{K}(\hat{\phi}, \hat{u})$, respectively, (4.6) can be rewritten as

$$\frac{1}{\epsilon_0} \int_\Omega (\hat{\varphi} - \phi_0) \psi \, d\Omega - \int_\Omega \sigma \operatorname{grad} \psi \cdot \operatorname{grad} \lambda \, d\Omega - \int_{\Gamma_C} f'(\hat{\phi}) \, \psi \lambda \, d\Gamma = 0 \quad \forall \, \psi \in H^1(\Omega)$$

which is clearly equivalent to (4.4). Equations (4.7)–(4.8) implies that, for all $u \in U$,

$$\frac{1}{2\epsilon_0}\int_\Omega (\hat\phi-\phi_0)^2\,d\Omega + \frac{\delta_0}{2}\int_{\Gamma_C}\hat u^2\,d\Gamma$$
$$-\left[\int_\Omega \sigma\,\mathrm{grad}\,\hat\phi\cdot\mathrm{grad}\,\lambda\,d\Omega + \int_{\Gamma_C} f(\hat\phi)\lambda\,d\Gamma - \int_{\Gamma_A}\hat u\,\lambda\,d\Gamma\right]$$
$$\le \frac{1}{\epsilon_0}\int_\Omega (\hat\phi-\phi_0)^2\,d\Omega + \frac{\delta_0}{2}\int_{\Gamma_C} u^2\,d\Gamma$$
$$-\left[\int_\Omega \sigma\,\mathrm{grad}\,\hat\phi\cdot\mathrm{grad}\,\lambda\,d\Omega + \int_{\Gamma_C} f(\hat\phi)\lambda\,d\Gamma - \int_{\Gamma_A} u\,\lambda\,d\Gamma\right],$$

i.e.,

$$\frac{\delta_0}{2}\int_{\Gamma_C}(u-\hat u)(u+\hat u)\,d\Gamma + \int_{\Gamma_A}(u-\hat u)\,\lambda\,d\Gamma \ge 0 \quad \forall\, u\in U. \tag{4.9}$$

Given any $w \in U$ and $\epsilon \in (0,1)$, we set $u = (1-\epsilon)\hat u + \epsilon w$ in (4.9) (note $u \in U$ due to the convexity of U) and obtain

$$\frac{\delta_0}{2}\int_{\Gamma_C}\epsilon\,(w-\hat u)(\epsilon w - \epsilon\hat u + 2\hat u)\,d\Gamma + \int_{\Gamma_A}\epsilon\,(w-\hat u)\,\lambda\,d\Gamma \ge 0 \quad \forall\, w\in U.$$

Thus (4.5) follows by dividing the last inequality by ϵ and then letting $\epsilon \to 0^+$. ∎

5. An Optimality System And The Regularity Of Its Solutions

In the sequel we will treat the special case $U = L^2(\Gamma_A)$. From (4.5) we easily obtain

$$\hat u = -\frac{1}{\delta_0}\lambda. \tag{5.1}$$

From (4.4), (5.1) and the original constraint equation (1.7), we form the following system of equations (dispensing with the hat notations to denote optimal solutions):

$$\int_\Omega \sigma\,\mathrm{grad}\,\phi\cdot\mathrm{grad}\,\psi\,d\Omega + \int_{\Gamma_C} f(\phi)\psi\,d\Gamma = -\frac{1}{\delta_0}\int_{\Gamma_A}\lambda\,\psi\,d\Gamma, \quad \forall\,\psi\in H^1(\Omega) \tag{5.2}$$

and

$$\int_\Omega \sigma\,\mathrm{grad}\,\lambda\cdot\mathrm{grad}\,\omega\,d\Omega + \int_{\Gamma_C} f'(\phi)\lambda\,\omega\,d\Gamma = \frac{1}{\epsilon_0}\int_\Omega (\phi-\phi_0)\,\omega\,d\Omega, \quad \forall\,\omega\in H^1(\Omega). \tag{5.3}$$

This system of equations will be called the *optimality system.*

Integrations by parts may be used to show that the system (5.2)-(5.3) constitutes a weak formulation of the problem

$$-\,\mathrm{div}(\sigma\,\mathrm{grad}\,\phi) = 0 \quad \text{in } \Omega, \tag{5.4}$$

$$\sigma\frac{\partial\phi}{\partial n} = -\frac{1}{\delta_0}\lambda \quad \text{on } \Gamma_A, \quad \sigma\frac{\partial\phi}{\partial n} = 0 \quad \text{on } \Gamma_0 \quad \text{and} \quad \sigma\frac{\partial\phi}{\partial n} = -f(\phi) \quad \text{on } \Gamma_C, \tag{5.5}$$

$$-\operatorname{div}(\sigma \operatorname{grad} \lambda) = \frac{1}{\epsilon_0}(\phi - \phi_0) \quad \text{in } \Omega\,, \tag{5.6}$$

$$\sigma\frac{\partial \lambda}{\partial n} = 0 \quad \text{on } \Gamma_A \cup \Gamma_0 \qquad \text{and} \qquad \sigma\frac{\partial \lambda}{\partial n} = -f'(\phi)\lambda \quad \text{on } \Gamma_C\,, \tag{5.7}$$

Now we examine the regularity of solutions of the optimality system (5.2)–(5.3), or equivalently, (5.4)–(5.7).

Theorem 5.1 *Suppose that $\Omega \subset \mathbb{R}^2$ is convex or of class $C^{1,1}$. Assume $(\phi, \lambda) \in H^1(\Omega) \times H^1(\Omega)$ is a solution to the optimality system* (5.2)–(5.3)*, or equivalently,* (5.4)–(5.7)*, then we have that $(\phi, \lambda) \in W^{3/2,r}(\Omega) \times W^{3/2,r}(\Omega)$ for $r \in [1, \infty)$.*

Proof: Since ϕ, $\lambda \in H^1(\Omega)$, Lemma 2.3 implies $f(\phi) \in L^r(\Gamma_C)$ and $f'(\phi) \in L^r(\Gamma_C)$ for all $r \in [1, \infty)$. We infer from trace theorems that $\lambda \in L^q(\Gamma_C)$ for all $q > 1$. Hence we have $\sigma\frac{\partial\phi}{\partial n} \in L^q(\Gamma)$ and $\sigma\frac{\partial\lambda}{\partial n} \in L^q(\Gamma)$ for each $q > 1$. By applying elliptic regularity results to equations (5.4)–(5.7), we obtain $\phi \in W^{3/2,q}(\Omega)$ and $\lambda \in W^{3/2,q}(\Omega)$ for each $q > 1$.

Remark *In general the possible discontinuity of the normal derivative on the intersection of Γ_C, Γ_0 and Γ_A prohibits us from obtaining further regularity. However, if ϕ and λ vanish on the entire intersection of Γ_C, Γ_0 and Γ_A, then we could in fact show that $\phi \in C^2(\Omega) \cap C(\overline{\Omega})$ and $\lambda \in C^2(\Omega) \cap C(\overline{\Omega})$, i.e., ϕ and λ are in fact classical solutions of the optimality system. Also, $H^2(\Omega)$-regularity for ϕ and λ is expected.*

6. Finite Element Approximations

6.1 Finite Element Discretizations. A finite element discretization of the optimality system (5.2)–(5.3) is defined in the usual manner. For simplicity we assume the domain Ω is a convex polygon. We first choose families of finite dimensional subspaces $V^h \subset H^1(\Omega)$ satisfying the approximation property: there exists a constant C and an integer k such that

$$\|v - v^h\|_1 \le C h^m \|v\|_{m+1}\,, \quad \forall\, v \in H^{m+1}(\Omega)\,,\ 1 \le m \le k\,. \tag{6.1}$$

One may consult, *e.g.*, [3] or [6] for a catalogue of finite element spaces satisfying (6.1). Then, we may formulate the approximate problem for the optimality system (5.2)–(5.3): seek $\phi^h \in V^h$ and $\lambda^h \in V^h$ such that

$$\begin{aligned} \int_\Omega \sigma \operatorname{grad} \phi^h \cdot \operatorname{grad} \psi^h \, d\Omega + \int_{\Gamma_C} f(\phi^h)\psi^h \, d\Gamma \\ = -\frac{1}{\delta_0}\int_{\Gamma_A} \lambda^h \psi^h \, d\Gamma\,, \quad \forall\, \psi^h \in V^h \end{aligned} \tag{6.2}$$

and

$$\begin{aligned} \int_\Omega \sigma \operatorname{grad} \lambda^h \cdot \operatorname{grad} \omega^h \, d\Omega + \int_{\Gamma_C} f'(\phi^h)\lambda^h \omega^h \, d\Gamma \\ = \frac{1}{\epsilon_0}\int_\Omega (\phi^h - \phi_0)\omega^h \, d\Omega\,, \quad \forall\, \omega^h \in V^h\,. \end{aligned} \tag{6.3}$$

6.2. Quotation of Brezzi-Rappaz-Raviart Approximation Theory.

The error estimate to be derived in Section 6.3 makes use of results developed by Brezzi, Rappaz and Raviart (see [5], also [7] and [8]) concerning the approximation of a class of nonlinear problems. Here, for the sake of completeness, we will state the relevant results, specialized to our needs.

The nonlinear problems considered in [5] (also [7] and [8]) are of the type

$$F(\psi) \equiv \psi + TG(\psi) = 0 \tag{6.4}$$

where X and Y are Banach spaces and $T \in \mathcal{L}(Y;X)$, G is a C^2 mapping from X into Y. A solution ψ to the equation $F(\psi) = 0$ is called a *nonsingular solution* if we have that $F'(\psi)$ is an isomorphism from X into X. (Here, $F'(\cdot)$ denotes the Frechet derivative of $F(\cdot)$.)

Approximations are defined by introducing a family of finite dimensional subspaces $X^h \subset X$ and for each $h > 0$ an approximating operator $T^h \in \mathcal{L}(Y;X^h)$. Then, we seek $\psi^h \in X^h$ such that

$$F^h(\psi^h) \equiv \psi^h + T^h G(\psi^h) = 0\,. \tag{6.5}$$

We will assume that there exists another Banach space Z, contained in Y, with continuous imbedding, such that

$$G'(\psi) \in \mathcal{L}(X;Z) \quad \forall\, \psi \in X\,. \tag{6.6}$$

Concerning the operator T^h, we assume the approximation properties

$$\lim_{h\to 0} \|(T^h - T)y\|_X = 0 \quad \forall\, y \in Y \tag{6.7}$$

and

$$\lim_{h\to 0} \|(T^h - T)\|_{\mathcal{L}(Z;X)} = 0\,. \tag{6.8}$$

Note that (6.6) and (6.8) imply that the operator $G'(\psi) \in \mathcal{L}(X;X)$ is compact. Morevover, (6.8) follows from (6.7) whenever the imbedding $Z \subset Y$ is compact.

We can now state the first result that will be used in the sequel. In the statement of the theorem, G'' represents the second order Frechet derivative of G.

Theorem 6.1 *Let X and Y be Banach spaces. Assume that G is a second order Frechet differentiable mapping from X into Y and that G'' is bounded on all bounded sets of X. Assume that* (6.6)-(6.8) *hold and that ψ is a nonsingular solution of* (6.4). *Then, there exists a $\delta > 0$ and an $h_0 > 0$ such that for $h \leq h_0$, there exists a unique $\psi^h \in X^h$ satisfying ψ^h is a nonsingular solution of* (6.5) *and $\|\psi^h - \psi\|_X \leq \delta$. Moreover, there exists a constant $C > 0$, independent of h, such that*

$$\|\psi^h - \psi\|_X \leq C\|(T^h - T)G(\psi)\|_X \quad \blacksquare \tag{6.9}$$

For the second result, we need to introduce two other Banach spaces H and W, such that $W \subset X \subset H$, with continuous imbeddings, and assume that

> *for all $w \in W$, the operator $G'(w)$ may be extended as a linear operator of $\mathcal{L}(H;Y)$, the mapping $w \to G'(w)$ being continuous* from W onto $\mathcal{L}(H;Y)$. (6.10)

We also suppose that

$$\lim_{h\to 0} \|T^h - T\|_{\mathcal{L}(Y;H)} = 0. \tag{6.11}$$

Then we may state the following additional result.

Theorem 6.2 *Assume that the hypotheses of Theorem* 6.1 *hold and that* (6.10) *and* (6.11) *hold. Assume further that*

$$F'(\psi) \text{ is an isomorphism of } H. \tag{6.12}$$

Then, for $h \le h_1$ sufficiently small, there exists a constant C, independent of h, such that

$$\|\psi^h - \psi\|_H \le C\|(T^h - T)G(\psi)\|_H + \|\psi^h - \psi\|_X^2. \quad \blacksquare \tag{6.13}$$

6.3 Error Estimates for the Approximations of Solutions of the Optimality System.

In order to derive error estimates, we begin by recasting the optimality system (5.2)–(5.3) and its discretization (6.2)–(6.3) into a form that fits into the framework of *Brezzi-Rappaz-Raviart* theory summarized in §6.2.

We define

$$X = H^1(\Omega) \times H^1(\Omega),$$

$$Y = H^{-1/2}(\Gamma) \times H^1(\Omega)^* \times H^{-1/2}(\Gamma),$$

$$Z = L^2(\Gamma) \times L^2(\Omega) \times L^2(\Gamma)$$

and

$$X^h = V^h \times V^h,$$

where $H^1(\Omega)^*$ denotes the dual space of $H^1(\Omega)$. Note that using Sobolev imbedding theorems, $Z \subset Y$ with a compact imbedding.

Let the operator $T \in \mathcal{L}(Y;X)$ be defined in the following manner: $T(\zeta,\eta,\theta) = (\phi,\lambda)$ for $(\zeta,\eta,\theta) \in Y$ and $(\phi,\lambda) \in X$ if and only if

$$\int_\Omega \sigma \,\mathrm{grad}\,\phi \cdot \mathrm{grad}\,\psi \, d\Omega + \alpha \int_{\Gamma_C} \phi\psi \, d\Gamma = \langle \zeta, \psi\rangle_\Gamma, \quad \forall\, \psi \in H^1(\Omega) \tag{6.14}$$

and

$$\int_\Omega \sigma \,\mathrm{grad}\,\lambda \cdot \mathrm{grad}\,\omega \, d\Omega + \alpha \int_{\Gamma_C} \lambda\,\omega \, d\Gamma = \langle \eta, \omega\rangle + \langle \theta, \omega\rangle_\Gamma, \quad \forall\, \omega \in H^1(\Omega). \tag{6.15}$$

Clearly, (6.14)–(6.15) consists of two *uncoupled* elliptic equations with mixed Robin-Neumann type boundary conditions and T is its solution operator.

Analogously, the operator $T^h \in \mathcal{L}(Y;X^h)$ is defined as follows: $T^h(\zeta,\eta,\theta) = (\phi^h,\lambda^h)$ for $(\zeta,\eta,\theta) \in Y$ and $(\phi^h,\lambda^h) \in X^h$ if and only if

$$\int_\Omega \sigma \,\mathrm{grad}\,\phi^h \cdot \mathrm{grad}\,\psi^h \, d\Omega + \alpha \int_{\Gamma_C} \phi^h\psi^h \, d\Gamma = \langle \zeta, \psi^h\rangle_\Gamma, \quad \forall\, \psi^h \in V^h \tag{6.16}$$

and

$$\int_\Omega \sigma \operatorname{grad} \lambda^h \cdot \operatorname{grad} \omega^h \, d\Omega + \alpha \int_{\Gamma_C} \lambda^h \omega^h \, d\Gamma = \langle \eta, \omega^h \rangle + \langle \theta, \omega^h \rangle_\Gamma \,, \quad \forall\, \omega^h \in V^h \,. \tag{6.17}$$

Clearly, (6.16)–(6.17) consists of two discrete Poisson-type equations that are discretizations of the equations (6.14)–(6.15); also, T^h is the solution operator for these two discrete equations.

By the well-known results concerning the approximation of elliptic equations (see, *e.g.*, [3] or [6]), we obtain:

$$\|(T - T^h)(\zeta, \eta, \theta)\|_X \to 0 \quad \text{as } h \to 0 \,, \tag{6.18}$$

for all $(\zeta, \eta, \theta) \in Y$ and, in addition, if $T(\zeta, \eta, \theta) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then

$$\|(T - T^h)(\zeta, \eta, \theta)\|_X \le C h^m \|T(\zeta, \eta, \theta)\|_{H^{m+1}(\Omega) \times H^{m+1}(\Omega)} \,. \tag{6.19}$$

Also, because $Z \subset Y$ with a compact imbedding, we have that

$$\|(T - T^h)\|_{\mathcal{L}(Z;X)} \to 0 \quad \text{as } h \to 0 \,. \tag{6.20}$$

Next, we define the *nonlinear* mapping $G: X \to Y$ as follows: $G(\phi, \lambda) = (\zeta, \eta, \theta)$ for $(\phi, \lambda) \in X$ and $(\zeta, \eta, \theta) \in Y$ if and only if

$$\langle \zeta, \pi \rangle_\Gamma = \frac{1}{\delta_0} \int_{\Gamma_A} \lambda \pi \, d\Gamma + \int_{\Gamma_C} (f(\phi) - \alpha \phi) \pi \, d\Gamma \quad \forall\, \pi \in H^{1/2}(\Gamma) \,, \tag{6.21}$$

$$\langle \eta, \omega \rangle = -\frac{1}{\epsilon_0} \int_\Omega (\phi - \phi_0)\, \omega \, d\Omega \quad \forall\, \omega \in H^1(\Omega) \tag{6.22}$$

and

$$\langle \theta, \tau \rangle_\Gamma = \int_{\Gamma_C} (f'(\phi) - \alpha) \lambda \, \tau \, d\Gamma \quad \forall\, \tau \in H^{1/2}(\Gamma) \,. \tag{6.23}$$

(6.21)-(6.23) is equivalent to

$$\zeta = \begin{cases} \frac{1}{\delta_0} \lambda & \text{on } \Gamma_A \,; \\ f(\phi) - \alpha \phi & \text{on } \Gamma_C \,; \\ 0 & \text{on } \Gamma_0 \,, \end{cases} \tag{6.24}$$

$$\eta = -\frac{1}{\epsilon_0} (\phi - \phi_0) \quad \text{in } \Omega \tag{6.25}$$

and

$$\theta = \begin{cases} (f'(\phi) - \alpha) \lambda & \text{on } \Gamma_C \,; \\ 0 & \text{on } \Gamma_0 \cup \Gamma_A \,. \end{cases} \tag{6.26}$$

Recall $f(\phi) = C_3(e^{C_1 \phi} - e^{C_2 \phi})$ so that $f'(\phi) = C_3(C_1 e^{C_1 \phi} + C_2 e^{C_2 \phi})$. Using Lemma 2.2 and trace theorems we infer that if $(\phi, \lambda) \in H^1(\Omega) \times H^1(\Omega)$, then for all $q > 1$,

$\phi|_\Gamma \in L^q(\Gamma)$, $\lambda|_\Gamma \in L^q(\Gamma)$, $f(\phi) \in L^q(\Gamma)$ and $f'(\phi) \in L^q(\Gamma)$. Hence we see that the triplet (ζ, η, θ) defined by (6.24)-(6.26) is indeed in Y, *i.e.*, G is well-defined.

It is easily seen that the optimality system (5.2)–(5.3) is equivalent to

$$(\phi, \lambda) + TG(\phi, \lambda) = 0 \tag{6.27}$$

and that the discrete optimality system (6.2)–(6.3) is equivalent to

$$(\phi^h, \lambda^h) + T^h G(\phi^h, \lambda^h) = 0\,. \tag{6.28}$$

We have thus recast our continuous and discrete optimality problems into a form that enables us to apply the theories of §6.2. It remains to verify the hypotheses in Theorem 6.1. This will be the task of the next two propositions.

Proposition 6.3 *The operator $G : X \to Y$ defined by* (6.21)-(6.23) *is second order Frechet differentiable. Furthermore,* (6.6) *holds and G'' is bounded on all bounded sets of X.*

Proof. In showing the differentiability of G, the linear terms appearing in the definition of G does not pose any difficulty. Furthermore the nonlinear terms in (6.21) and (6.23) can be dealt with in a similar way. For clarity, we will only analyse the differentiability of the nonlinear term $\tau \mapsto \int_{\Gamma_C} f'(\phi)\lambda\tau\, d\Gamma$. We define a mapping $Q : X \to H^{-1/2}(\Gamma)$ by $\langle Q(\phi, \lambda), \tau\rangle \equiv \int_{\Gamma_C} f'(\phi)\lambda\tau\, d\Gamma$ for all $(\phi, \lambda) \in X$ and $\tau \in H^{1/2}(\Gamma)$. For each given $(\phi, \lambda) \in X$ we have that

$$\begin{aligned}
&\Big\langle Q(\phi+\delta\phi, \lambda+\delta\lambda) - Q(\phi,\lambda), \tau\Big\rangle \\
&\qquad\qquad - \int_{\Gamma_C} f''(\phi)(\delta\phi)\,\lambda\tau\, d\Gamma - \int_{\Gamma_C} f'(\phi)(\delta\lambda)\tau\, d\Gamma \\
&= \int_{\Gamma_C} [f'(\phi+\delta\phi) - f'(\phi) - f''(\phi)(\delta\phi)]\,\lambda\tau\, d\Gamma \\
&\qquad\qquad + \int_{\Gamma_C} [f'(\phi+\delta\phi) - f'(\phi)](\delta\lambda)\tau\, d\Gamma \\
&= \int_{\Gamma_C}\int_0^1 [f''\big((1-t)\phi + t(\phi+\delta\phi)\big) - f''(\phi)]\, dt\,(\delta\phi)\,\lambda\tau\, d\Gamma + \\
&\qquad + \int_{\Gamma_C}\int_0^1 f''\big((1-t)\phi + t(\phi+\delta\phi)\big)\, dt\,(\delta\phi)(\delta\lambda)\tau\, d\Gamma \\
&= \int_{\Gamma_C}\int_0^1\int_0^1 t\, f'''\big(s(1-t)\phi + st(\phi+\delta\phi) + (1-s)\phi\big)\, ds\, dt\, |\delta\phi|^2\,\lambda\tau\, d\Gamma \\
&\quad + \int_{\Gamma_C}\int_0^1 f''\big((1-t)\phi + t(\phi+\delta\phi)\big)\, dt\,(\delta\phi)(\delta\lambda)\tau\, d\Gamma \quad \forall\,(\delta\phi,\delta\lambda)\in X.
\end{aligned} \tag{6.29}$$

Note that $f(\phi) = C_3(e^{C_1\phi} - e^{-C_2\phi})$, $f'(\phi) = C_3(C_1 e^{C_1\phi} + C_2 e^{-C_2\phi})$, $f''(\phi) = C_3(C_1^2 e^{C_1\phi} - C_2^2 e^{-C_2\phi})$ and $f'''(\phi) = C_3(C_1^3 e^{C_1\phi} + C_2^3 e^{-C_2\phi})$. By Lemma 2.2 we have that for all real number $m > 1$,

$$\|f'(\phi)\|_{L^m(\Gamma_C)} \le C\, \Big\{1 + |\Gamma| + e^{\,m^2 C\|\phi\|_1^2}\, |\Gamma|\Big\}^{\frac{1}{m}}\,,$$

$$\|f''(\phi)\|_{L^m(\Gamma_C)} \leq C\left\{1+|\Gamma|+e^{\;m^2C\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}$$

and

$$\|f'''(\phi)\|_{L^m(\Gamma_C)} \leq C\left\{1+|\Gamma|+e^{\;m^2C\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}},$$

where C is a generic constant independent of ϕ. Trace theorems for $\Omega \subset \mathbf{R}^2$ implies that for all $p>1$, $q>1$ and $r>1$,

$$\|\delta\phi\|_{L^p(\Gamma_C)} \leq C\|\delta\phi\|_1 \quad \forall\,\delta\phi \in H^1(\Omega),$$

$$\|\delta\lambda\|_{L^q(\Gamma_C)} \leq C\|\delta\lambda\|_1 \quad \forall\,\delta\lambda \in H^1(\Omega)$$

and

$$\|\tau\|_{L^r(\Gamma_C)} \leq C\|\tau\|_{1/2,\Gamma} \quad \forall\,\tau \in H^{1/2}(\Gamma).$$

We fix some $m>1$, $p>1$, $q>1$ and $r>1$ with $\frac{1}{m}+\frac{1}{p}+\frac{1}{q}+\frac{1}{r}=1$. Then for every $(\delta o, \delta\lambda) \in X$ we have that

$$\begin{aligned}
&\int_{\Gamma_C}\int_0^1 f''\big((1-t)\phi+t(\phi+\delta\phi)\big)\,dt\,(\delta\phi)(\delta\lambda)\tau\,d\Gamma \leq \\
&\leq \sup_{0\leq t\leq 1}\|f''\big((1-t)\phi+t(\phi+\delta\phi)\big)\|_{L^m(\Gamma_C)}\,\|\delta\phi\|_{L^p(\Gamma_C)}\,\|\delta\lambda\|_{L^q(\Gamma_C)}\,\|\tau\|_{L^r(\Gamma_C)} \\
&\leq C\left\{1+|\Gamma|+e^{m^2 2C\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}\,\|\delta\phi\|_1\,\|\delta\lambda\|_1\,\|\tau\|_{1/2,\Gamma} \quad \forall\,\tau \in H^{1/2}(\Gamma).
\end{aligned}$$

Similarly, we have that for every $\delta\phi \in H^1(\Omega)$ and every $\tau \in H^{1/2}(\Gamma)$,

$$\begin{aligned}
&\int_{\Gamma_C}\int_0^1\int_0^1 t\,f'''\big(s(1-t)\phi+st(\phi+\delta\phi)+(1-s)\phi\big)\,ds\,dt\,|\delta\phi|^2\,\lambda\tau\,d\Gamma \leq \\
&\leq C\left\{1+|\Gamma|+e^{m^2 3C\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}\,\|\delta\phi\|_1^2\,\|\lambda\|_1\,\|\tau\|_{1/2,\Gamma}\,.
\end{aligned}$$

Returning to (6.29) we obtain that for all $\tau \in H^{1/2}(\Gamma)$ and $(\delta\phi, \delta\lambda) \in X$,

$$\begin{aligned}
&\Big\langle Q(\phi+\delta\phi,\lambda+\delta\lambda)-Q(\phi,\lambda),\tau\Big\rangle - \int_{\Gamma_C} f''(\phi)(\delta\phi)\,\lambda\tau\,d\Gamma - \int_{\Gamma_C} f'(\phi)(\delta\lambda)\tau\,d\Gamma \leq \\
&\leq C\left\{1+|\Gamma|+e^{m^2 3C\|\phi\|_1^2}\,|\Gamma|\right\}^{\frac{1}{m}}\left\{\|\delta\phi\|_1\,\|\delta\lambda\|_1+\|\delta\phi\|_1^2\,\|\lambda\|_1\right\}\,\|\tau\|_{1/2,\Gamma}\,,
\end{aligned}$$

so that we conclude Q as a mapping from X to $H^{-1/2}(\Gamma)$ is Frechet differentiable and its derivative $Q'(\phi,\lambda)$ is given by

$$\Big\langle Q'(\phi,\lambda)(\tilde{\psi},\tilde{\omega}),\tau\Big\rangle = \int_{\Gamma_C}[f''(\phi)\tilde{\psi}\lambda\tau+f'(\phi)\tilde{\omega}\tau]\,d\Gamma \quad \forall\,\tau \in H^{1/2}(\Gamma).$$

Hence, taking into account the remarks in the beginning of the proof, we have justified that G is Frechet differentiable and its Frechet derivative $G'(\phi,\lambda)$ is defined

as follows. For each $(\phi,\lambda) \in X$, $G'(\phi,\lambda)(\tilde{\psi},\tilde{\omega}) = (\tilde{\zeta},\tilde{\eta},\tilde{\theta})$ for $(\tilde{\psi},\tilde{\omega}) \in X$ and $(\tilde{\zeta},\tilde{\eta},\tilde{\theta}) \in Y$ if and only if

$$\langle\tilde{\zeta},\pi\rangle_\Gamma = \frac{1}{\delta_0}\int_{\Gamma_A} \tilde{\omega}\,\pi\,d\Gamma + \int_{\Gamma_C} (f'(\phi)\tilde{\psi} - \alpha\tilde{\psi})\pi\,d\Gamma \quad \forall\,\pi \in H^{1/2}(\Gamma), \tag{6.30}$$

$$\langle\tilde{\eta},\omega\rangle = -\frac{1}{\epsilon_0}\int_\Omega \tilde{\psi}\,\omega\,d\Omega \quad \forall\,\omega \in H^1(\Omega) \tag{6.31}$$

and

$$\langle\tilde{\theta},\tau\rangle_\Gamma = \int_{\Gamma_C} f''(\phi)\tilde{\psi}\lambda\,\tau\,d\Gamma + \int_{\Gamma_C} (f'(\phi)-\alpha)\tilde{\omega}\,\tau\,d\Gamma \quad \forall\,\tau \in H^{1/2}(\Gamma); \tag{6.32}$$

or, equivalently,

$$\tilde{\zeta} = \begin{cases} \frac{1}{\delta_0}\tilde{\omega} & \text{on } \Gamma_A\,; \\ f'(\phi)\tilde{\psi} - \alpha\tilde{\psi} & \text{on } \Gamma_C\,; \\ 0 & \text{on } \Gamma_0\,, \end{cases} \tag{6.33}$$

$$\tilde{\eta} = -\frac{1}{\epsilon_0}\tilde{\psi} \quad \text{in } \Omega \tag{6.34}$$

and

$$\tilde{\theta} = \begin{cases} f''(\phi)\lambda\tilde{\psi} + (f'(\phi)-\alpha)\tilde{\omega} & \text{on } \Gamma_C\,; \\ 0 & \text{on } \Gamma_0 \cup \Gamma_A\,. \end{cases} \tag{6.35}$$

(These defining equations can be formally derived by differentiating (6.21)–(6.23).) It is easy to verify from the above equations that for each $(\tilde{\psi},\tilde{\omega}) \in X$, we have $(\tilde{\zeta},\tilde{\eta},\tilde{\theta}) \in Z$, *i.e.*, $G'(\phi,\lambda)$ maps X into Z; furthermore, using trace theorems and Lemma 2.2 we obtain that

$$\begin{aligned}\|\tilde{\zeta}\|_{0,\Gamma} &\le \frac{1}{\delta_0}\|\tilde{\omega}\|_{0,\Gamma} + \|f'(\phi)\|_{L^4(\Gamma_C)}\,\|\tilde{\psi}\|_{L^4(\Gamma)} + \alpha\|\tilde{\psi}\|_{0,\Gamma} \\ &\le \frac{C}{\delta_0}\|\tilde{\omega}\|_1 + C\left\{1 + |\Gamma| + e^{C\|\phi\|_1^2}\,|\Gamma|\right\}^{1/4}\|\tilde{\psi}\|_1 + C\|\tilde{\psi}\|_1\,,\end{aligned}$$

$$\|\tilde{\eta}\|_0 \le \frac{1}{\epsilon}\|\tilde{\psi}\|_1$$

and

$$\begin{aligned}&\|\tilde{\zeta}\|_{0,\Gamma} \le \|f''(\phi)\|_{L^6(\Gamma_C)}\,\|\tilde{\psi}\|_{L^6(\Gamma)}\,\|\lambda\|_{L^6(\Gamma)} + \|f'(\phi)\|_{L^4(\Gamma_C)}\,\|\tilde{\omega}\|_{L^4(\Gamma)} + \alpha\|\tilde{\omega}\|_{0,\Gamma} \\ &\le C\left\{1 + |\Gamma| + e^{C\|\phi\|_1^2}\,|\Gamma|\right\}^{1/4}\{\|\tilde{\psi}\|_1\,\|\lambda\|_1 + \|\tilde{\omega}\|_1\} + C\|\tilde{\omega}\|_1\,.\end{aligned}$$

Thus $G'(\phi,\lambda) \in \mathcal{L}(X;Z)$, *i.e.*, we have shown that (6.6) hold.

To show the second order differentiability of G, again for clarity we will examine only one nonlinear term appearing in the definition of G', *e.g.*, the term $\tau \mapsto \int_{\Gamma_C} f''(\phi)\tilde{\psi}\lambda\tau\,d\Gamma$. We define a mapping $R : X \to \mathcal{L}(X; H^{-1/2}(\Gamma))$ by

$\left\langle R(\phi,\lambda)(\tilde\psi,\tilde\omega),\tau\right\rangle \equiv \int_{\Gamma_C} f''(\phi)\tilde\psi\lambda\tau\, d\Gamma$ for all (ϕ,λ), $(\tilde\psi,\tilde\omega)\in X$ and $\tau\in H^{1/2}(\Gamma)$. For each given $(\phi,\lambda)\in X$ we have that for all $(\delta\phi,\delta\lambda)\in X$,

$$\begin{aligned}
&\Big\langle [R(\phi+\delta\phi,\lambda+\delta\lambda)-R(\phi,\lambda)](\tilde\psi,\tilde\omega),\tau\Big\rangle \\
&\qquad\qquad -\int_{\Gamma_C} f'''(\phi)(\delta\phi)\tilde\psi\,\lambda\tau\,d\Gamma - \int_{\Gamma_C} f''(\phi)\tilde\psi(\delta\lambda)\tau\,d\Gamma \\
&= \int_{\Gamma_C} [f''(\phi+\delta\phi)-f''(\phi)-f'''(\phi)(\delta\phi)]\tilde\psi\,\lambda\tau\,d\Gamma \\
&\qquad\qquad + \int_{\Gamma_C} [f''(\phi+\delta\phi)-f''(\phi)]\tilde\psi(\delta\lambda)\tau\,d\Gamma \\
&= \int_{\Gamma_C}\int_0^1\int_0^1 t\,f''''(s(1-t)\phi+st(\phi+\delta\phi)+(1-s)\phi)\,ds\,dt\,\tilde\psi|\delta\phi|^2\,\lambda\tau\,d\Gamma \\
&\qquad\qquad + \int_{\Gamma_C}\int_0^1 f'''((1-t)\phi+t(\phi+\delta\phi))\,dt\,(\delta\phi)(\delta\lambda)\tilde\psi\tau\,d\Gamma\,.
\end{aligned}$$

Thus similar to the analysis ensuing (6.29), we can show that the operator R is Frechet differentiable and its derivative $R'(\phi,\lambda)$ is defined by:

$$R'(\phi,\lambda)\cdot\big((\tilde\psi,\tilde\omega),(\tilde{\tilde\psi},\tilde{\tilde\omega})\big) = \int_{\Gamma_C} f'''(\phi)\,\tilde{\tilde\phi}\,\tilde\psi\,\lambda\,\tau\,d\Gamma + \int_{\Gamma_C} f''(\phi)\,\tilde\psi\,\tilde{\tilde\lambda}\,\tau\,d\Gamma\,.$$

Hence, G is second order Frechet differentiable and $G''(\phi,\lambda)$ is defined as follows. For each $(\phi,\lambda)\in X$, $G''(\phi,\lambda)\cdot\big((\tilde\psi,\tilde\omega),(\tilde{\tilde\psi},\tilde{\tilde\omega})\big)=(\tilde\zeta,\tilde\eta,\tilde\theta)$ for $\big((\tilde\psi,\tilde\omega),(\tilde{\tilde\psi},\tilde{\tilde\omega})\big)\in X\times X$ and $(\tilde\zeta,\tilde\eta.\tilde\theta)\in Y$ if and only if

$$\langle\tilde\zeta,\pi\rangle_\Gamma = \int_{\Gamma_C} f''(\phi)\,\tilde{\tilde\psi}\,\tilde\psi\,\pi\,d\Gamma \quad \forall\,\pi\in H^{1/2}(\Gamma)\,,$$

$$\langle\tilde\eta,\omega\rangle = 0 \quad \forall\,\omega\in H_0^1(\Omega)$$

and

$$\langle\tilde\theta,\tau\rangle_\Gamma = \int_{\Gamma_C}[f'''(\phi)\,\tilde{\tilde\psi}\,\tilde\psi\,\lambda + f''(\phi)\,\tilde\psi\,\tilde{\tilde\lambda}]\,\tau\,d\Gamma + \int_{\Gamma_C} f''(\phi)\,\tilde{\tilde\psi}\,\tilde\omega\,\tau\,d\Gamma \quad \forall\,\tau\in H^{1/2}(\Gamma)\,;$$

or, equivalently,

$$\tilde\zeta = \begin{cases} 0 & \text{on } \Gamma_A\,; \\ f''(\phi)\tilde{\tilde\psi}\,\tilde\psi & \text{on } \Gamma_C\,; \\ 0 & \text{on } \Gamma_0\,, \end{cases} \tag{6.36}$$

$$\tilde\eta = 0 \quad \text{in } \Omega \tag{6.37}$$

and

$$\tilde\theta = \begin{cases} [f'''(\phi)\tilde{\tilde\psi}\,\tilde\psi\,\lambda + f''(\phi)\tilde\psi\,\tilde{\tilde\lambda}] + f''(\phi)\tilde{\tilde\psi}\,\tilde\omega & \text{on } \Gamma_C\,; \\ 0 & \text{on } \Gamma_0\cup\Gamma_A\,. \end{cases} \tag{6.38}$$

Furthermore, using Lemma 2.2, (6.36)-(6.38) and trace theorems, we may derive a bound for $G''(\phi,\lambda)$ for each given (ϕ,λ):

$$||G''(\phi,\lambda)||_Y \le C\left\{1+|\Gamma|+e^{C\|\phi\|_1^2}|\Gamma|\right\}(1+\|\lambda\|_1)$$

for some constant C, so that G'' is bounded on every bounded subset of X. ∎

A solution (ϕ,λ) of the problem (5.2)–(5.3), or equivalently, of (6.27), is nonsingular if the *linear system*

$$\begin{aligned}\int_\Omega \sigma \operatorname{grad}\tilde{\phi}\cdot\operatorname{grad}\psi\,d\Omega + \int_{\Gamma_C} f'(\phi)\tilde{\phi}\psi\,d\Gamma \\ + \frac{1}{\delta_0}\int_{\Gamma_A}\tilde{\lambda}\psi\,d\Gamma = \langle\tilde{\zeta},\psi\rangle \quad \forall\,\psi\in H^1(\Omega)\end{aligned} \tag{6.39}$$

and

$$\begin{aligned}\int_\Omega \sigma \operatorname{grad}\tilde{\lambda}\cdot\operatorname{grad}\omega\,d\Omega + \int_{\Gamma_C} f''(\phi)\,\tilde{\phi}\,\lambda\,\omega\,d\Gamma + \int_{\Gamma_C} f'(\phi)\,\tilde{\lambda}\,\omega\,d\Gamma \\ - \frac{1}{\epsilon_0}\int_\Omega \tilde{\phi}\,\omega\,d\Omega = \langle\tilde{\eta},\omega\rangle \quad \forall\,\omega\in H^1(\Omega)\end{aligned} \tag{6.40}$$

has a unique solution $(\tilde{\phi},\tilde{\lambda})\in X$ for every $\tilde{\zeta},\tilde{\eta}\in H^1(\Omega)^*$.

An analogous definition holds for nonsingular solutions of the discrete optimality system (6.2)–(6.3), or equivalently, (6.28).

It is evident that (6.39)-(6.40) has a unique solution for large enough σ, *e.g.*,

$$\sigma > \max\left\{\frac{C}{\delta_0},\ \frac{C}{\epsilon_0},\ C\|\lambda\|_{L^4(\Gamma_C)}\,\|f''(\phi)\|_{L^4(\Gamma_C)}\right\}.$$

It is reasonable to assume that (6.39)-(6.40) has a unique solution generically with respect to σ, *i.e.*, the optimal solutions are almost always nonsingular. Thus Theorem 6.1 and Proposition 6.3 lead to the following:

Theorem 6.4 *Assume* (ϕ,λ) *is a nonsingular solution of the optimality system* (5.2)-(5.3). *Assume that the finite element spaces* V^h *satisfy the condition* (6.1). *Then, there exists a* $\delta>0$ *and* $h_0>0$ *such that for* $h\le h_0$, *there exists a unique nonsigular solution* (ϕ^h,λ^h) *of the discrete optimality system* (6.2)-(6.3) *satisfying* $\|\phi^h-\phi\|_1+\|\lambda^h-\lambda\|_1\le\delta$. *Moreover,*

$$\|\phi^h-\phi\|_1+\|\lambda^h-\lambda\|_1\to 0 \quad as\ h\to 0\,. \tag{6.41}$$

If, in addition, the solution of the optimality system satisfies $(\phi,\lambda)\in H^{m+1}(\Omega)\times H^{m+1}(\Omega)$, *then there exists a constant* C, *independent of* h, *such that*

$$\|\phi-\phi^h\|_1+\|\lambda-\lambda^h\|_1\le Ch^m\big(\|\phi\|_{m+1}+\|\lambda\|_{m+1}\big)\,. \quad ∎ \tag{6.42}$$

A consequence of Theorems 6.4 is the following corollary that gives error estimates for the approximation of the controls.

Corollary 6.5 *Assume (ϕ, λ) is a nonsingular solution of the optimality system (5.2)-(5.3). Assume that the finite element spaces V^h satisfy the condition (6.1). Define the approximate control by*

$$u^h = -\frac{1}{\delta_0}\lambda^h \quad \text{on } \Gamma_A .$$

Then

$$\|u^h - u\|_{1/2,\Gamma_A} \to 0 \quad \text{as } h \to 0 . \tag{6.43}$$

If, in addition, the solution of the optimality system satisfies $(\phi, \lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then there exists a constant C, independent of h, such that for $h \le h_0$,

$$\|u^h - u\|_{1/2,\Gamma_A} \le \frac{C}{\delta_0} h^m \left(\|\phi\|_{m+1} + \|\lambda\|_{m+1}\right) . \tag{6.44}$$

Proof: Recall that $u = -\frac{1}{\delta_0}\lambda$ on Γ_A; see (5.1). Then (6.43) and (6.44) follow trivially from (6.41)-(6.42) and the inequalities (see [1])

$$\|u - u^h\|_{1/2,\Gamma_A} = \frac{1}{\delta_0}\|\lambda - \lambda^h\|_{1/2,\Gamma_C} \le \frac{1}{\delta_0}\|\lambda - \lambda^h\|_{1/2,\Gamma} \le \frac{C}{\delta_0}\|\lambda - \lambda^h\|_1 . \quad \blacksquare$$

Now we wish to apply Theorem 6.2 to derive $L^2(\Gamma_C)$-error estimates for the approximations of u. To this end, we assume the domain Ω is convex and for each given $\epsilon \in (0, 1/4)$, we introduce spaces

$$H = H^{1/2+\epsilon}(\Omega) \times H^{1/2+\epsilon}(\Omega) \qquad \text{and} \qquad W = H^{3/2+\epsilon}(\Omega) \times H^{3/2+\epsilon}(\Omega) .$$

Note that $X \subset H$ with a compact imbedding so that (6.18) implies

$$\|(T - T^h)\|_{\mathcal{L}(Y;H)} \to 0 \quad \text{as } h \to 0 .$$

Again using finite element approximation results in [6] we have that if Ω is convex and $T(\zeta, \eta, \theta) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then

$$\|(T - T^h)(\zeta, \eta, \theta)\|_H \le C h^{m-\epsilon+1/2} \|T(\zeta, \eta, \theta)\|_{H^{m+1}(\Omega) \times H^{m+1}(\Omega)} .$$

Proposition 6.6 *For each $(\phi, \lambda) \in W$, the operator $G'(\phi, \lambda) : X \to Y$ defined by (6.33)-(6.35) can be extended as a linear operator of $\mathcal{L}(H; Y)$. Furthermore, the mapping $w \to G'(w)$ is continuous from W onto $\mathcal{L}(H; Y)$.*

Proof. Note that $W \subset L^\infty(\Omega) \times L^\infty(\Omega)$ and $H^{1/2+\epsilon}(\Omega)|_\Gamma \subset L^2(\Gamma)$ with continuous imbeddings. For each $(\phi, \lambda) \in W$, we can easily verify from (6.33)-(6.35) that

$$\begin{aligned}
&\|G'(\phi, \lambda)(\tilde{\psi}, \tilde{\omega})\|_Y \\
&\le A(\phi)\left\{\|\tilde{\omega}\|_{0,\Gamma_A} + \|\tilde{\psi}\|_{0,\Gamma_C} + \|\tilde{\psi}\|_0 + \|\tilde{\omega}\|_{0,\Gamma_C}\right\} \\
&\le C_T A(\phi)\left\{\|\tilde{\omega}\|_{1/2+\epsilon} + \|\tilde{\psi}\|_{1/2+\epsilon}\right\} \quad \forall\, (\tilde{\psi}, \tilde{\omega}) \in H ,
\end{aligned}$$

where

$$A(\phi) = C \max\left\{ \frac{1}{\delta_0}, \frac{1}{\epsilon_0}, \max_{|\mathbf{x}|\leq\|\phi\|_{3/2+\epsilon}} (|f'(\mathbf{x})| + \alpha), \max_{|\mathbf{x}|\leq\|\phi\|_{3/2+\epsilon}} (|f''(\mathbf{x})| \, \|\lambda\|_{3/2+\epsilon}) \right\}$$

and C_T is a constant such that $\|\psi\|_{0,\Gamma} \leq C_T \|\psi\|_{1/2+\epsilon}$ for all $\psi \in H^{1/2+\epsilon}(\Omega)$. The desired results follow easily from this estimate. ∎

If (ϕ, λ) is a nonsingular solution of (5.2)-(5.3), using the denseness of $H^1(\Omega)$ in $H^{1/2+\epsilon}(\Omega)$ and regularity theories for (6.39)-(6.40), we infer that (6.12) holds.

Thus we have verified all the requirements in Theorem 6.2 so that we can draw the following conclusion:

Theorem 6.7 *Assume Ω is convex and (ϕ, λ) is a nonsingular solution of the optimality system* (5.2)-(5.3). *Assume that the finite element spaces V^h satisfy the condition* (6.1). *Then, there exists a $\delta > 0$ and $h_0 > 0$ such that for $h \leq h_0$, there exists a unique nonsingular solution (ϕ^h, λ^h) of the discrete optimality system* (6.2)-(6.3) *satisfying $\|\phi^h - \phi\|_1 + \|\lambda^h - \lambda\|_1 \leq \delta$. If, in addition, the solution of the optimality system satisfies $(\phi, \lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then there exists a constant C, independent of h, such that*

$$\|\phi - \phi^h\|_{\epsilon+1/2} + \|\lambda - \lambda^h\|_{\epsilon+1/2} \leq C h^{m-\epsilon+1/2} (\|\phi\|_{m+1} + \|\lambda\|_{m+1}) \,. \quad ∎ \tag{6.45}$$

A consequence of Theorem 6.7 is the following corollary that gives the $L^2(\Gamma_A)$-error estimates for the the approximation of the controls.

Corollary 6.8 *Assume Ω is convex and (ϕ, λ) is a nonsingular solution of the optimality system* (5.2)-(5.3). *Assume that the finite element spaces V^h satisfy the condition* (6.1). *Define the approximate control by*

$$u^h = -\frac{1}{\delta_0} \lambda^h \quad \text{on } \Gamma_A \,.$$

If the solution of the optimality system satisfies $(\phi, \lambda) \in H^{m+1}(\Omega) \times H^{m+1}(\Omega)$, then for each $\epsilon \in (0, 1/4)$ there exists a constant C, independent of h, such that for $h \leq h_0$,

$$\|u^h - u\|_{0,\Gamma_A} \leq \frac{C}{\delta_0} h^{m-\epsilon+1/2} (\|\phi\|_{m+1} + \|\lambda\|_{m+1}) \,. \tag{6.46}$$

Proof: Recall that $u = -\frac{1}{\delta_0}\lambda$ on Γ_A; see (5.1). Then (6.46) follows trivially from (6.45) and the trace theorems (see [1])

$$\|u - u^h\|_{0,\Gamma_A} = \frac{1}{\delta_0} \|\lambda - \lambda^h\|_{0,\Gamma_C} \leq \frac{1}{\delta_0} \|\lambda - \lambda^h\|_{0,\Gamma} \leq \frac{C}{\delta_0} \|\lambda - \lambda^h\|_{\epsilon+1/2} \,. \quad ∎$$

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